IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated. Part 6. C_8H_8–C_8H_{10} Hydrocarbons with Water

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The mutual solubility and related liquid-liquid equilibria of C_8H_8–C_8H_{10} hydrocarbons with water are exhaustively and critically reviewed. Reports of experimental determination of solubility in 5 chemically distinct binary systems that appeared in the primary literature prior to the end of 2002 are compiled. For all the systems sufficient data are available to allow critical evaluation. All data are expressed as mass percent and mole fraction as well as the originally reported units. In addition to the standard evaluation criteria used throughout the Solubility Data Series, a new method based on the evaluation of all experimental data for a given homologous series of aliphatic and aromatic hydrocarbons was used. [DOI: 10.1063/1.1839880]

Key words: C_8H_8–C_8H_{10} hydrocarbons; critical evaluation; liquid-liquid equilibria; solubility; water

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*A Critical Evaluation is prepared for this system.

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1. Preface

1.1. Scope of this Volume

This paper is Part 6 of a revised and updated version of an earlier compilation and evaluation of the mutual solubility of water and hydrocarbon compounds containing five or more carbon atoms (Shaw[1,2]). This new work incorporates the compilations prepared for the original version (with correction of typographical and other errors where such have been discovered) together with new compilations based on recent and previously overlooked reports in the peer-reviewed scientific literature prior to 2003. To facilitate comparison of data, all original results are expressed in terms of mass percent and mole fraction as well as the units reported by the original investigators.

This revised work also includes all new evaluations for systems where two or more independent measurements of solubility have been reported. In these evaluations reported solubility values are characterized as Recommended, Tentative, Doubtful, or Rejected, based on consistency between independently determined experimental values and reference values derived from a newly developed set of smoothing equations.[3–6] Recommended values are supported by two (or more) independent experimental values and a reference value that are all in agreement. Tentative values are supported by two (or more) independent values in agreement with each other, but not with the reference value, or one experimental

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value in agreement with the reference value. Doubtful values are those for which a single experimental value differs from the reference value. Experimental values that differ from reference values and other experimental values are Rejected.

Detailed introductory material including explanations of the formats of compilation and evaluation, definitions of commonly used measures of solubility, and the scope of the Solubility Data Series can be found in Part 1 (Goral *et al.*[6]). The derivation of the smoothing equations used for calculate reference values can be found in Parts 1 and 2 (Maczynski and Shaw[7,8]).

1.2. References for the Preface

[1] D. Shaw, Editor, IUPAC Solubility Data Series, Vol. 37, *Hydrocarbons with Water and Seawater, Part I: Hydrocarbons C_5 to C_7* (Pergamon, New York, 1989).

[2] D. Shaw, Editor, IUPAC Solubility Data Series, Vol. 38, *Hydrocarbons with Water and Seawater, Part II: Hydrocarbons C_8 to C_{36}* (Pergamon, New York, 1989).

[3] A. Maczynski, M. Goral, B. Wisniewska-Goclowska, A. Skrzecz, and D. Shaw, Monatshefte Chemie **134**, 633 (2003).

[4] A. Maczynski, B. Wisniewska-Goclowska, and M. Goral, Recommended Liquid-Liquid Equilibrium Data. Part 1. Binary Alkane-Water Systems, J. Phys. Chem. Ref. Data **33**, 549 (2004).

[5] M. Goral, A. Maczynski, and B. Wisniewska-Goclowska, Recommended Liquid-Liquid Equilibrium Data. Part 2. Binary Unsaturated Hydrocarbon-Water Systems, J. Phys. Chem. Ref. Data. **33**, 579 (2004).

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[7] A. Maczynski and D. Shaw, Editors, IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated. Part 1. C_5 Hydrocarbons with Water, J. Phys. Chem. Ref. Data **34**, 441 (2005).

[8] A. Maczynski and D. Shaw, Editors, IUPAC-NIST Solubility Data Series. 81. Hydrocarbons with Water and Seawater—Revised and Updated. Part 2. Benzene with Water and Heavy Water, J. Phys. Chem. Ref. Data **34**, 477 (2005).

2. C_8H_8–C_8H_{10} Hydrocarbons with Water

2.1. Styrene+Water

Components:
(1) Styrene; C_8H_8; [100-42-5]
(2) Water; H_2O; [7732-18-5]

Evaluators:
A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, January, 2004.

Critical Evaluation of the Solubility of Styrene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

Author (s)	T/K	Author (s)	T/K
Andrews and Keefer[1]	298	Fordyce and Chapin[4]	333
Banerjee *et al.*[2]	298	Lane[5]	280–338
Frilette and Hohenstein[3]	298		

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 2 and expressed by the equation:

$$\ln x_1 = \ln x_{\min,1} + D[(T_{\min}/T)\ln(T_{\min}/T) + 1 - (T_{\min}/T)], \quad (1)$$

where $\ln x_{\min,1} = -9.90$, $D = 61.8$, and $T_{\min} = 290$ K. The parameters $\ln x_{\min,1}$ and D were individually adjusted to solubility of styrene because it is somewhat more soluble than alkylbenzenes due to additional double bond.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the Reference data. Comparison between Reference and experimental data is one of the criteria used to assign data to categories.

All the experimental and reference data are listed in Table 1 and shown in Fig. 1. The data of Andrews and Keefer,[1] and Lane[5] at 298 K are in good agreement (within 30% relative standard deviation) with each other and with the reference data and are Recommended. All other data of Lane[5] and the data of Frilette and Hohenstein[3] at 298 K are in good agreement with the reference data (within 30% relative standard deviation) and are Tentative. The data of Banerjee *et al.*[2] at 298 K, and Fordyce and Chapin[4] at 333 K are in poor agreement (greater than 30% relative standard deviation) with the reference data and are Doubtful.

TABLE 1. Experimental values for solubility of styrene (1) in water (2)

T/K	Experimental values x_1 (R=recommended, T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
280.2	$5.00 \cdot 10^{-5}$ (T; Ref. 5)	$5.2 \cdot 10^{-5}$
288.2	$4.30 \cdot 10^{-5}$ (T; Ref. 5)	$5.0 \cdot 10^{-5}$
297.2	$5.70 \cdot 10^{-5}$ (T; Ref. 5)	$5.1 \cdot 10^{-5}$
298.2	$5.19 \cdot 10^{-5}$ (R; Ref. 1), $2.77 \cdot 10^{-5}$ (D; Ref. 2), $3.80 \cdot 10^{-5}$ (T; Ref. 3), $5.30 \cdot 10^{-5}$ (R; Ref. 5)	$5.1 \cdot 10^{-5}$
305.2	$6.20 \cdot 10^{-5}$ (T; Ref. 5)	$5.4 \cdot 10^{-5}$
313.2	$6.90 \cdot 10^{-5}$ (T; Ref. 5)	$5.9 \cdot 10^{-5}$
317.2	$6.90 \cdot 10^{-5}$ (T; Ref. 5)	$6.3 \cdot 10^{-5}$
322.2	$7.80 \cdot 10^{-5}$ (T; Ref. 5)	$6.9 \cdot 10^{-5}$
324.2	$7.80 \cdot 10^{-5}$ (T; Ref. 5)	$7.1 \cdot 10^{-5}$
329.2	$8.60 \cdot 10^{-5}$ (T; Ref. 5)	$7.9 \cdot 10^{-5}$
333.5	$1.66 \cdot 10^{-3}$ (D; Ref. 4)	$8.7 \cdot 10^{-5}$
338.2	$1.00 \cdot 10^{-4}$ (T; Ref. 5)	$9.7 \cdot 10^{-5}$

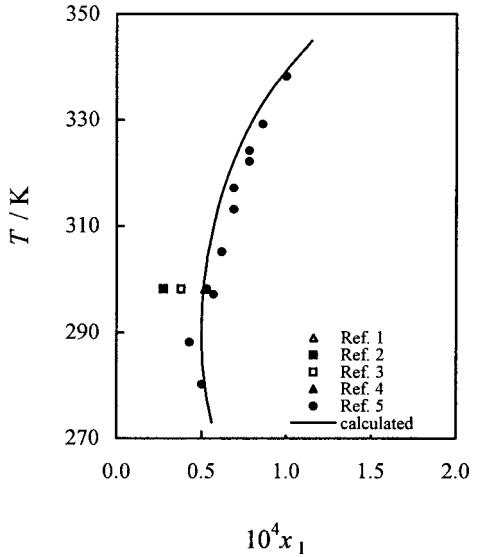

FIG. 1. All the solubility data for styrene (1) in water (2).

Critical Evaluation of the Solubility of Water (2) in Styrene (1)

The experimental solubility for (2) on (1) have been investigated by Lane[5] at 279 K–324 K. Reference solubility data for (2) in (1) were obtained by the Evaluators using the method described in the Preface to Part 2 and expressed by the equation:

$$\ln x_2 = d_1 + d_2(1/T_r - 1) + d_3(1 - T_r)^{1/3} + d_4(1 - T_r), \quad (2)$$

where $d_1 = -0.314$, $d_2 = -0.910$, $d_3 = 2.643$, $d_4 = -13.598$, and $T_r = T/576.1$.

Equation (2) was used for obtaining the Reference data by regression of the data obtained from those calculated from Reference data of solubility of styrene in water by the Equation of State with an association term. Comparison between Reference and experimental data is one of the criteria used to assign data to categories.

All the experimental and reference solubility data for (2) in (1) are listed in Table 2 and shown in Fig. 2. All the data are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative.

TABLE 2. Experimental values for solubility of water (2) in styrene (1)

T/K	Experimental values x_2 (T=tentative)	Reference values $x_2 \pm 30\%$
279.2	$1.8 \cdot 10^{-3}$ (T; Ref. 5)	$2.1 \cdot 10^{-3}$
287.2	$2.3 \cdot 10^{-3}$ (T; Ref. 5)	$2.6 \cdot 10^{-3}$
298.2	$3.8 \cdot 10^{-3}$ (T; Ref. 5)	$3.5 \cdot 10^{-3}$
300.2	$3.5 \cdot 10^{-3}$ (T; Ref. 5)	$3.7 \cdot 10^{-3}$
304.2	$4.8 \cdot 10^{-3}$ (T; Ref. 5)	$4.1 \cdot 10^{-3}$
307.2	$4.6 \cdot 10^{-3}$ (T; Ref. 5)	$4.5 \cdot 10^{-3}$
313.2	$5.8 \cdot 10^{-3}$ (T; Ref. 5), $5.7 \cdot 10^{-3}$ (T; Ref. 5)	$5.2 \cdot 10^{-3}$
318.2	$6.9 \cdot 10^{-3}$ (T; Ref. 5)	$6.0 \cdot 10^{-3}$
324.2	$7.1 \cdot 10^{-3}$ (T; Ref. 5)	$7.0 \cdot 10^{-3}$

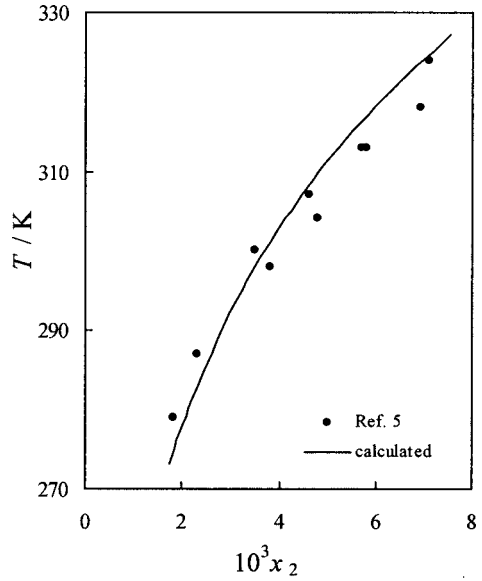

FIG. 2. All the solubility data for water (2) in styrene (1).

References:

[1]L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **72**, 5034 (1950).

[2]S. Banerjee, S. H. Yalkowsky, and S. C. Valvani, Environ. Sci. Technol. **14**, 1227 (1980).

[3]V. J. Frilette and W. P. Hohenstein, J. Polym. Sci. **3**, 22 (1948).

[4]R. G. Fordyce and E. C. Chapin, J. Am. Chem. Soc. **69**, 581 (1947).

[5]W. H. Lane, Ind. Eng. Chem., Anal. Ed. **18**, 295 (1946).

Components:	**Original Measurements:**
(1) Styrene; C_8H_8; [100-42-5] (2) Water; H_2O; [7732-18-5]	S. Banerjee, S. H. Yalkowsky, and S. C. Valvani, Environ. Sci. Technol. **14**, 1227 (1980).
Variables:	**Prepared By:**
One temperature: 25 °C	G. T. Hefter

Experimental Data

The solubility of styrene in water was reported to be $1.54 \cdot 10^{-3}$ mol/L sln.

Assuming a solution density of 1.00 kg/L the corresponding mass percent and mole fraction (x_1) solubilities, calculated by the compiler, are 0.0160 $g(1)$/100 g sln and $2.77 \cdot 10^{-5}$, respectively.

Auxiliary Information

Method/Apparatus/Procedure:

Experiments were performed in sealed stainless steel centrifuge tubes. An excess of styrene was added to a tube containing distilled water, and the tube was sealed and allowed to equilibrate at 25±0.2 °C with constant or intermittent shaking. Equilibration was generally complete within 1 week. The mixture was then centrifuged at 10 000 rpm for 60 min in a head preequilibrated to 25±0.3 °C, following which aliquots of the solution were removed for analysis by high-performance liquid chromatography using a Waters M6000A instrument fitted with a C18 Bondapak column. The mobile phase was a mixture of methanol/water or acetonitrile/water. The entire procedure was carried out at least twice for each compound, and each analysis was also conducted in duplicate.

Source and Purity of Materials:

(1) Aldrich; purity not specified.
(2) Distilled.

Estimated Error:

Temperature: ±0.2 °C.
Solubility: ±5.7% rel. (representing 1 standard deviation).

Components:	**Original Measurements:**
(1) Styrene; C_8H_8; [100-42-5] (2) Water; H_2O; [7732-18-5]	L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **72**, 5034 (1950).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and Z. Maczynska

Experimental Data

The solubility of styrene in water at 25 °C was reported to be 0.030 $g(1)$/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is $5.19 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of (1) and (2) was rotated for 20 h in a constant temperature bath as 25 °C. A sample (5–20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10–50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

Source and Purity of Materials:

(1) Eastman Kodak Co. white label; distilled shortly before use; 1 wt % of hydroquinone added as stabilizer before distillation; boiling point 76 °C (78 mm Hg).
(2) Not specified.

Estimated Error:

Not specified.

Components:	**Original Measurements:**
(1) Styrene; C_8H_8; [100-42-5] (2) Water; H_2O; [7732-18-5]	V. J. Frilette and W. P. Hohenstein, J. Polym. Sci. **3**, 22 (1948).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and Z. Maczynska

Experimental Data

The solubility of styrene in water at 25 °C was reported to be 0.022 $g(1)$/100 g sln.

The corresponding mole fraction, x_1, value calculated by the compilers is $3.8 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:

The saturated solutions of (1) in (2) were prepared in two different ways. In the first method, conjugated solutions were prepared by shaking together excess (1) with (2) and allowing the layers to separate; the aqueous layer was then analyzed for (1). To avoid the possibility of contaminating the aqueous phase by small suspended droplets a second method was utilized; a cellophane sack, filled with (2) was completely submerged in a beaker containing (2); a layer of (1) was then floated on top of (2) in the beaker. After 48 h at 25 °C the sack was retrieved and the contents carefully removed and analyzed.

The method of analysis was not described.

Source and Purity of Materials:

(1) Not specified.
(2) Distilled.

Estimated Error:

Not specified.

Components:
(1) Styrene; C_8H_8; [100-42-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. G. Fordyce and E. C. Chapin, J. Am. Chem. Soc. **69**, 581 (1947).

Variables:
One temperature: 60.3 °C

Prepared By:
A. Maczynski

Experimental Data

The solubility of styrene in water at 60.3 °C was reported to be 0.96 $g(1)$/100 g(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.95 $g(1)$/100 g sln and $1.66 \cdot 10^{-3}$.

Auxiliary Information

Method/Apparatus/Procedure:
Into two stoppered 50 mL Erlenmeyer flasks were weighed two 25.000 g portions of (2). The flasks were placed in water bath regulated to 60.3 ± 0.02 °C. Component (1) was added a drop at a time to the water samples by means of a calibrated micro-pipet and the flasks agitated after each addition. The saturation point was taken at the first appearance of the turbidity and amount of (1) was calculated from the number of drops added.

Source and Purity of Materials:
(1) Dow Chemical Co., N-100; redistilled.
(2) Not specified.

Estimated Error:
Temperature: ± 0.02 °C.
Solubility: ± 0.05 $g(1)$/100 g sln.

Components:
(1) Styrene; C_8H_8; [100-42-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. H. Lane, Ind. Eng. Chem., Anal. Ed. **18**, 295 (1946).

Variables:
Temperature: 7 °C–65 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

Solubility of styrene in water

(a) Formaldehyde-Sulfuric Acid Reagent Method

t/°C	$10^5 \cdot x_1$ (compiler)	$g(1)$/100 g sln
7	5.0	0.029
24	5.7	0.033
32	6.2	0.036
40	6.9	0.040
51	7.8	0.045

Solubility of styrene in water

(b) Cloud Point Method

t/°C	$10^5 \cdot x_1$ (compiler)	$g(1)$/100 g sln
15	4.3	0.025
25	5.3	0.031
44	6.9	0.040
49	7.8	0.045
56	8.6	0.050
65	10.0	0.058

Auxiliary Information

Method/Apparatus/Procedure:
(a) The solubility of (1) in (2) was determined by means of the formaldehyde-sulfuric acid reagent, Morris *et al.*[1] The value shown for 7 °C is the mean of three determinations, and the value for 25 °C is the mean of two determinations; all other data are single determinations only.

(b) The cloud point exhibited by this system appeared to be very sharp, as the samples passed from a state in which they were cloudy within 1 °C. The cloud point data averages of from two to eight separate determinations. Cloud points at 0.025 $g(1)$/100 g solution were very faint.

Source and Purity of Materials:
(1) Source not specified; fresh samples; used as received.
(2) Not specified.

Estimated Error:
Temperature: (b) ± 0.5 °C (from two to eight determinations).

References:
[1]H. E. Morris, R. B. Stiles, and W. H. Lane, Ind. Eng. Chem. Anal. Ed. **18**, 294 (1946).

Components:	**Original Measurements:**
(1) Styrene; C_8H_8; [100-42-5] (2) Water; H_2O; [7732-18-5]	W. H. Lane, Ind. Eng. Chem., Anal. Ed. **18**, 295 (1946).
Variables:	**Prepared By:**
Temperature: 6 °C–51 °C	A. Maczynski and Z. Maczynska

Experimental Data

Solubility of water in styrene

(a) Karl Fischer Reagent Method

t/°C	$10^3 \cdot x_2$ (compiler)	$g(2)$/100 g sln
6	1.8	0.032
24	3.8	0.066
31	4.8	0.084
40	5.8	0.101
51	7.1	0.123

Solubility of water in styrene

(b) Cloud Point Method

t/°C	$10^3 \cdot x_2$ (compiler)	$g(2)$/100 g sln
14	2.3	0.040
27	3.5	0.060
34	4.6	0.080
49	5.7	0.100
45	6.9	0.120

Auxiliary Information

Method/Apparatus/Procedure:

(a) A large sample of (1) containing a slight excess of (2) was shaken at a given temperature and then allowed to stand in a water bath at this temperature for 24 h to ensure complete separation of the two phases before withdrawal of sample of the (1) rich phase for titration of the water present with Karl Fischer reagent.
(b) Duplicate determinations gave cloud points agreeing within 1 °C, except in case of 0.120 $g(1)$/100 g sln where the agreement was within 3 °C. Cloud points at 0.040 $g(1)$/100 g sln were very faint. No more details were reported.

Source and Purity of Materials:

(1) Source not specified; fresh samples; used as received.
(2) Not specified.

Estimated Error:

Temperature: (b) ±1 to ±3 °C.
Solubility: (a) ±1.5% (from two determinations).

2.2. Ethylbenzene+Water

Components:	**Evaluators:**
(1) Ethylbenzene; C_8H_{10}; [100-41-4] (2) Water; H_2O; [7732-18-5]	A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, January, 2004.

Critical Evaluation of the Solubility of Ethylbenzene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below together with temperature range and pressure range, if reported:

Author (s)	T/K	Author (s)	T/K
Andrews and Keefer[1]	298	McAuliffe[20]	298
Ben-Naim and Wilf[2]	298	Morrison and Billett[21]	298
Ben-Naim and Wilf[3]	283–293	Owens *et al.*[22]	283–318
Bohon and Claussen[4]	298	Polak and Lu[23]	273 and 298
Brown and Wasik[5]	278–293	Price[24]	298
Chen and Wagner[6]	303–373 (136–204 kPa)	Sanemasa *et al.*[25]	288–318
Dohanyosova *et al.*[7]	274–328	Sanemasa *et al.*[26]	288–318
Fühner[10]	288	Sanemasa *et al.*[27]	298
Guseva and Parnov[11]	388–507	Sanemasa *et al.*[28]	298
Heidman *et al.*[13]	312–553 (111–8590 kPa)	Sawamura *et al.*[29]	298
Jones and Monk[14]	298–308	Sawamura *et al.*[30]	273–323
Keeley *et al.*[15]	298	Schwarz and Miller[31]	283–293
Klevens[16]	288	Sutton and Calder[32]	298
Korenman and Aref'eva[17]	293	Tewari *et al.*[33]	298
Korenman and Aref'eva[18]	298	Vesala[34]	298
McAuliffe[19]	298		

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 2 and expressed by the equation:

$$\ln x_1 = \ln x_{\min,1} + D[(T_{\min}/T)\ln(T_{\min}/T) + 1 - (T_{\min}/T)], \quad (1)$$

where $\ln x_{\min,1} = -10.37$, $D = 40.9$, and $T_{\min} = 290$.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the Reference data. Comparison between Reference and experimental data is one of the criteria used to assign data to the categories listed in Table 3.

TABLE 3. The data categories for solubility of ethylbenzene (1) in water (2)

T/K	Recommended [data in good agreement (±30%) with each other and with the reference data]	Tentative [data in good agreement (±30%) with the reference data]	Doubtful data in poor agreement (>30%) with the reference data]
273.2	Polak and Lu[23], Sawamura *et al.*[30]		
273.7		Dohanyosova *et al.*[7]	
277.7		Brown and Wasik[5]	
278.2		Dohanyosova *et al.*[7], Sawamura *et al.*[30]	
279.5		Brown and Wasik[5]	
280.3		Brown and Wasik[5]	
282.2		Brown and Wasik[5]	
283.2	Ben-Naim and Wilf[2], Owens *et al.*[22], Schwarz and Miller[31]	Sawamura *et al.*[30], Schwarz and Miller[31]	
285.0		Brown and Wasik[5]	
285.3		Brown and Wasik[5]	
287.2		Owens *et al.*[22]	
288.2	Dohanyosova *et al.*[7], Klevens[16], Sawamura *et al.*[30]	Fühner[10], Sanemasa *et al.*[26]	Sanemasa *et al.*[25]
288.3		Brown and Wasik[5]	
290.2		Owens *et al.*[22]	
291.1		Brown and Wasik[5]	
291.2		Owens *et al.*[22]	
292.2		Owens *et al.*[22]	
293.2	Ben-Naim and Wilf[2], Korenman and Aref'eva[17], Owens *et al.*[22], Sawamura *et al.*[30], Schwarz and Miller[31]		
293.3		Brown and Wasik[5]	
294.2		Owens *et al.*[22]	
295.2		Owens *et al.*[22]	
296.7		Owens *et al.*[22]	
298.0		Vesala[34]	
298.1		Sanemasa *et al.*[28]	
298.2	Andrews and Keefer[1], Ben-Naim and Wilf[3], Bohon and Claussen[4], Dohanyosova *et al.*[7], Keeley *et al.*[15], Korenman and Aref'eva[18], McAuliffe[19], McAuliffe[20], Morrison and Billett[21], Owens *et al.*[22], Polak and Lu[23], Sanemasa *et al.*[26], Sanemasa *et al.*[27], Sawamura *et al.*[29], Sawamura *et al.*[30], Sutton and Calder[32], Tewari *et al.*[33]		Price,[24] Sanemasa *et al.*[25]
299.0		Owens *et al.*[22]	
301.2		Owens *et al.*[22]	
303.2	Chen and Wagner[6], Owens *et al.*[22], Sawamura *et al.*[30]		
308.2	Dohanyosova *et al.*[7], Owens *et al.*[22], Sanemasa *et al.*[26], Sawamura *et al.*[30]		Sanemasa *et al.*[25]
311.5			Heidman *et al.*[13]
313.2	Owens *et al.*[22], Sawamura *et al.*[30]	Chen and Wagner[6]	
318.2	Dohanyosova *et al.*[7], Owens *et al.*[22], Sanemasa *et al.*[26], Sawamura *et al.*[30]		Sanemasa *et al.*[25]
323.2		Chen and Wagner[6], Sawamura *et al.*[30]	
328.2		Dohanyosova *et al.*[7]	
333.2		Chen and Wagner[6]	
343.2		Chen and Wagner[6]	
353.2		Chen and Wagner[6]	
363.2		Chen and Wagner[6]	
367.6			Heidman *et al.*[13]
373.2		Chen and Wagner[6]	
388.2			Guseva and Parnov[11]
413.7		Guseva and Parnov[11]	
423.4			Heidman *et al.*[13]
443.7		Guseva and Parnov[11]	
479.5			Heidman *et al.*[13]
483.2		Guseva and Parnov[11]	
506.7		Guseva and Parnov[11]	
536.1			Heidman *et al.*[13]
552.8			Heidman *et al.*[13]

All the experimental and reference data are listed in Table 4 and shown in Fig. 3. The Recommended and Tentative data are shown in Fig. 4.

TABLE 4. Experimental values for solubility of ethylbenzene (1) in water (2)

T/K	P/kPa	Experimental values x_1 (R=recommended, T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
273.2		$3.34 \cdot 10^{-5}$ (R; Ref. 23), $3.234 \cdot 10^{-5}$ (R; Ref. 30)	$3.4 \cdot 10^{-5}$
273.7		$2.86 \cdot 10^{-5}$ (T; Ref. 7)	$3.4 \cdot 10^{-5}$
277.7		$3.33 \cdot 10^{-5}$ (T; Ref. 5)	$3.3 \cdot 10^{-5}$
278.2		$2.83 \cdot 10^{-5}$ (T; Ref. 7), $3.084 \cdot 10^{-5}$ (T; Ref. 30)	$3.3 \cdot 10^{-5}$
279.5		$3.26 \cdot 10^{-5}$ (T; Ref. 5)	$3.2 \cdot 10^{-5}$
280.3		$3.16 \cdot 10^{-5}$ (T; Ref. 5)	$3.2 \cdot 10^{-5}$
282.2		$3.18 \cdot 10^{-5}$ (T; Ref. 5)	$3.2 \cdot 10^{-5}$
283.2		$3.44 \cdot 10^{-5}$ (R; Ref. 2), $3.33 \cdot 10^{-5}$ (R; Ref. 22), $2.964 \cdot 10^{-5}$ (T; Ref. 30), $3.58 \cdot 10^{-5}$ (T; Ref. 31), $3.05 \cdot 10^{-5}$ (R; Ref. 31)	$3.2 \cdot 10^{-5}$
285.0		$3.07 \cdot 10^{-5}$ (T; Ref. 5)	$3.2 \cdot 10^{-5}$
285.3		$3.11 \cdot 10^{-5}$ (T; Ref. 5)	$3.2 \cdot 10^{-5}$
287.2		$3.27 \cdot 10^{-5}$ (T; Ref. 22)	$3.2 \cdot 10^{-5}$
288.2		$2.82 \cdot 10^{-5}$ (R; Ref. 7), $2.4 \cdot 10^{-5}$ (T; Ref. 10), $2.90 \cdot 10^{-5}$ (R; Ref. 16), $2.99 \cdot 10^{-4}$ (D; Ref. 25), $2.72 \cdot 10^{-5}$ (T; Ref. 26), $2.88 \cdot 10^{-5}$ (R; Ref. 30)	$3.1 \cdot 10^{-5}$
288.3		$3.06 \cdot 10^{-5}$ (T; Ref. 5)	$3.1 \cdot 10^{-5}$
290.2		$3.20 \cdot 10^{-5}$ (T; Ref. 22)	$3.1 \cdot 10^{-5}$
291.1		$3.12 \cdot 10^{-5}$ (T; Ref. 5)	$3.1 \cdot 10^{-5}$
291.2		$3.11 \cdot 10^{-5}$ (T; Ref. 22)	$3.1 \cdot 10^{-5}$
292.2		$3.02 \cdot 10^{-5}$ (T; Ref. 22)	$3.2 \cdot 10^{-5}$
293.2		$3.61 \cdot 10^{-5}$ (R; Ref. 2), $3.60 \cdot 10^{-5}$ (R; Ref. 17), $3.02 \cdot 10^{-5}$ (R; Ref. 22), $3.19 \cdot 10^{-5}$ (R; Ref. 22), $2.863 \cdot 10^{-5}$ (R; Ref. 30), $3.53 \cdot 10^{-5}$ (R; Ref. 31), $3.12 \cdot 10^{-5}$ (R; Ref. 31)	$3.2 \cdot 10^{-5}$
293.3		$3.10 \cdot 10^{-5}$ (T; Ref. 5)	$3.2 \cdot 10^{-5}$
294.2		$3.11 \cdot 10^{-5}$ (T; Ref. 22)	$3.2 \cdot 10^{-5}$
295.2		$3.09 \cdot 10^{-5}$ (T; Ref. 22)	$3.2 \cdot 10^{-5}$
296.7		$3.16 \cdot 10^{-5}$ (T; Ref. 22)	$3.2 \cdot 10^{-5}$
298.0		$3.44 \cdot 10^{-5}$ (T; Ref. 34)	$3.2 \cdot 10^{-5}$
298.1		$2.48 \cdot 10^{-5}$ (T; Ref. 28)	$3.2 \cdot 10^{-5}$
298.2	100 (Ref. 29)	$2.85 \cdot 10^{-5}$ (R; Ref. 1), $3.61 \cdot 10^{-5}$ (R; Ref. 3), $3.53 \cdot 10^{-5}$ (R; Ref. 4), $2.89 \cdot 10^{-5}$ (R; Ref. 7), $3.00 \cdot 10^{-5}$ (R; Ref. 15), $3.12 \cdot 10^{-5}$ (R; Ref. 18), $2.70 \cdot 10^{-5}$ (R; Ref. 19), $2.57 \cdot 10^{-5}$ (R; Ref. 20), $2.80 \cdot 10^{-5}$ (R; Ref. 21), $3.27 \cdot 10^{-5}$ (R; Ref. 22), $3.00 \cdot 10^{-5}$ (R; Ref. 23), $2.22 \cdot 10^{-5}$ (D; Ref. 24), $3.09 \cdot 10^{-4}$ (D; Ref. 25), $2.87 \cdot 10^{-5}$ (R; Ref. 26), $2.92 \cdot 10^{-5}$ (R; Ref. 27), $3.25 \cdot 10^{-5}$ (R; Ref. 29), $2.88 \cdot 10^{-5}$ (R; Ref. 30), $2.73 \cdot 10^{-5}$ (R; Ref. 32), $3.18 \cdot 10^{-5}$ (R; Ref. 33)	$3.2 \cdot 10^{-5}$
299.0		$3.17 \cdot 10^{-5}$ (T; Ref. 22)	$3.2 \cdot 10^{-5}$
301.2		$3.16 \cdot 10^{-5}$ (T; Ref. 22)	$3.2 \cdot 10^{-5}$
303.2	136 (Ref. 6)	$2.88 \cdot 10^{-5}$ (R; Ref. 6), $3.22 \cdot 10^{-5}$ (R; Ref. 22), $2.946 \cdot 10^{-5}$ (R; Ref. 30)	$3.3 \cdot 10^{-5}$
308.2		$3.02 \cdot 10^{-5}$ (R; Ref. 7), $3.29 \cdot 10^{-5}$ (R; Ref. 22), $3.31 \cdot 10^{-4}$ (D; Ref. 25), $2.99 \cdot 10^{-5}$ (R; Ref. 26), $3.047 \cdot 10^{-5}$ (R; Ref. 30)	$3.4 \cdot 10^{-5}$
311.5		$3.20 \cdot 10^{-4}$ (D; Ref. 13)	$3.5 \cdot 10^{-5}$
313.2	136 (Ref. 6)	$2.92 \cdot 10^{-5}$ (T; Ref. 6), $3.50 \cdot 10^{-5}$ (R; Ref. 22), $3.188 \cdot 10^{-5}$ (R; Ref. 30)	$3.5 \cdot 10^{-5}$
318.2		$3.23 \cdot 10^{-5}$ (T; Ref. 7), $3.62 \cdot 10^{-5}$ (T; Ref. 22), $3.69 \cdot 10^{-4}$ (D; Ref. 25), $3.33 \cdot 10^{-5}$ (T; Ref. 26), $3.338 \cdot 10^{-5}$ (T; Ref. 30)	$3.7 \cdot 10^{-5}$
323.2	136 (Ref. 6)	$3.35 \cdot 10^{-5}$ (T; Ref. 6), $3.525 \cdot 10^{-5}$ (T; Ref. 30)	$3.9 \cdot 10^{-5}$
328.2		$3.69 \cdot 10^{-5}$ (T; Ref. 7)	$4.2 \cdot 10^{-5}$
333.2	136 (Ref. 6)	$4.07 \cdot 10^{-5}$ (T; Ref. 6)	$4.5 \cdot 10^{-5}$
343.2	136 (Ref. 6)	$4.93 \cdot 10^{-5}$ (T; Ref. 6)	$5.3 \cdot 10^{-5}$
353.2	136 (Ref. 6)	$5.99 \cdot 10^{-5}$ (T; Ref. 6)	$6.3 \cdot 10^{-5}$
363.2	170 (Ref. 6)	$6.95 \cdot 10^{-5}$ (T; Ref. 6)	$7.7 \cdot 10^{-5}$

367.6	111 (Ref. 13)	$8.60\cdot10^{-4}$ (D; Ref. 13)	$8.4\cdot10^{-5}$
373.2	204 (Ref. 6)	$8.54\cdot10^{-5}$ (T; Ref. 6)	$9.4\cdot10^{-5}$
388.2		$8.71\cdot10^{-5}$ (D; Ref. 11)	$1.3\cdot10^{-4}$
413.7		$2.02\cdot10^{-4}$ (T; Ref. 11)	$2.4\cdot10^{-4}$
423.4	627 (Ref. 13)	$2.19\cdot10^{-3}$ (D; Ref. 13)	$3.1\cdot10^{-4}$
443.7		$6.04\cdot10^{-4}$ (T; Ref. 11)	$5.2\cdot10^{-4}$
479.5	2320 (Ref. 13)	$6.00\cdot10^{-3}$ (D; Ref. 13)	$1.3\cdot10^{-3}$
483.2		$1.13\cdot10^{-3}$ (T; Ref. 11)	$1.4\cdot10^{-3}$
506.7		$1.93\cdot10^{-3}$ (T; Ref. 11)	$2.6\cdot10^{-3}$
536.1	6500 (Ref. 13)	$3.25\cdot10^{-2}$ (D; Ref. 13)	$5.6\cdot10^{-3}$
552.8	8590 (Ref. 13)	$3.75\cdot10^{-2}$ (D; Ref. 13)	$8.5\cdot10^{-3}$

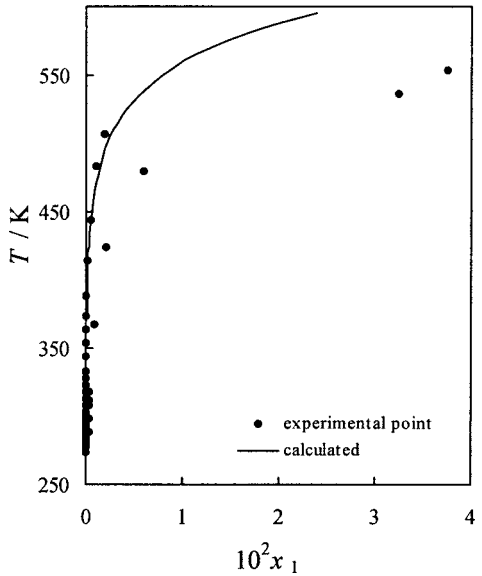

FIG. 3. All the solubility data for ethylbenzene (1) in water (2).

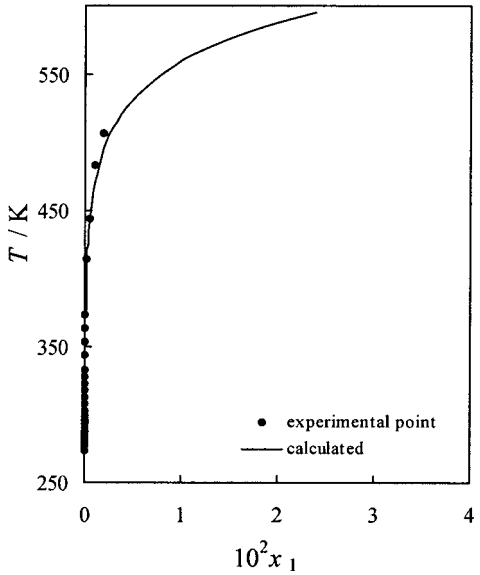

FIG. 4. Recommended and tentative solubility data for ethylbenzene (1) in water (2).

Critical Evaluation of the Solubility of Water (2) in Ethylbenzene (1)

The experimental solubility data for (2) in (1) have been investigated by the authors listed below together with temperature range and pressure range, if reported:

Author (s)	T/K	Author (s)	T/K
Chen and Wagner[6]	303–373 (136–204 kPa)	Heidman *et al.*[13]	312–553 (9–10 680 kPa)
Englin *et al.*[8]	283–303	Jones and Monk[14]	298–308
Filippov and Furman[9]	291–323	Polak and Lu[23]	273 and 298

Reference solubility data for (2) in (1) were obtained by the Evaluators using the method described in the Preface to Part 2 and expressed by the equation:

$$\ln x_2 = d_1 + d_2(1/T_r - 1) + d_3(1 - T_r)^{1/3} + d_4(1 - T_r), \quad (2)$$

where $d_1 = -0.383$, $d_2 = -3.167$, $d_3 = -0.009$, $d_4 = -5.655$, and $T_r = T/566.9$.

Equation (2) was used for obtaining the Reference data by regression of the data obtained from those calculated from Reference data of solubility of ethylbenzene in water by the Equation of State with an association term. Comparison between Reference and experimental data is one of the criteria used to assign data to the categories listed in Table 5.

TABLE 5. The data categories for solubility of water (2) in ethylbenzene (1)

T/K	Recommended [data in good agreement (±30%) with each other and with the reference data]	Tentative [data in good agreement (±30%) with the reference data]	Doubtful [data in poor agreement (>30%) with the reference data]
273.2		Polak and Lu[23]	
283.2		Englin *et al.*[8]	
291.4		Filippov and Furman[9]	
291.5		Filippov and Furman[9]	
292.9		Filippov and Furman[9]	
293.2		Englin *et al.*[8]	
295.5		Filippov and Furman[9]	
296.6		Filippov and Furman[9]	
297.4		Filippov and Furman[9]	
298.2	Jones and Monk[14] Polak and Lu[23]		
300.4		Filippov and Furman[9]	
303.0		Filippov and Furman[9]	
303.2	Chen and Wagner[6] Englin *et al.*[8] Jones and Monk[14]		
304.8		Filippov and Furman[9]	
305.3		Filippov and Furman[9]	
307.4		Filippov and Furman[9]	
308.2		Jones and Monk[14]	
308.3		Filippov and Furman[9]	
309.8			Filippov and Furman[9]
310.9		Heidman *et al.*[13]	
312.0			Filippov and Furman[9]
313.2		Chen and Wagner[6]	
314.7			Filippov and Furman[9]
316.3			Filippov and Furman[9]
320.4			Filippov and Furman[9]
322.7			Filippov and Furman[9]
323.2		Chen and Wagner[6]	
333.2		Chen and Wagner[6]	
343.2		Chen and Wagner[6]	
353.2		Chen and Wagner[6]	
363.2		Chen and Wagner[6]	
367.6		Heidman *et al.*[13]	
373.2		Chen and Wagner[6]	
423.4		Heidman *et al.*[13]	
479.5		Heidman *et al.*[13]	
536.1		Heidman *et al.*[13]	
550.4		Heidman *et al.*[13]	
568.1		Heidman *et al.*[13]	

The experimental and reference solubility data for (2) in (1) are listed in Table 6 and shown in Fig. 5. The Recommended and Tentative data are shown in Fig. 6.

TABLE 6. Experimental values for solubility of water (2) in ethylbenzene (1)

T/K	P/kPa	Experimental values x_2 (R=recommended, T=tentative, D=doubtful)	Reference values $x_2 \pm 30\%$
273.2		$1.05 \cdot 10^{-3}$ (T; Ref. 23)	$1.2 \cdot 10^{-3}$
283.2		$1.62 \cdot 10^{-3}$ (T; Ref. 8)	$1.7 \cdot 10^{-3}$
291.4		$1.74 \cdot 10^{-3}$ (T; Ref. 9)	$2.2 \cdot 10^{-3}$
291.5		$1.81 \cdot 10^{-3}$ (T; Ref. 9)	$2.2 \cdot 10^{-3}$
292.9		$1.92 \cdot 10^{-3}$ (T; Ref. 9)	$2.3 \cdot 10^{-3}$
293.2		$2.19 \cdot 10^{-3}$ (T; Ref. 8)	$2.3 \cdot 10^{-3}$
295.5		$2.07 \cdot 10^{-3}$ (T; Ref. 9)	$2.5 \cdot 10^{-3}$
296.6		$2.12 \cdot 10^{-3}$ (T; Ref. 9)	$2.5 \cdot 10^{-3}$
297.4		$2.28 \cdot 10^{-3}$ (T; Ref. 9)	$2.6 \cdot 10^{-3}$
298.2		$2.50 \cdot 10^{-3}$ (R; Ref. 14), $2.60 \cdot 10^{-3}$ (R; Ref. 23)	$2.7 \cdot 10^{-3}$
300.4		$2.91 \cdot 10^{-3}$ (T; Ref. 9)	$2.9 \cdot 10^{-3}$
303.0		$3.50 \cdot 10^{-3}$ (T; Ref. 9)	$3.1 \cdot 10^{-3}$
303.2	136 (Ref. 6)	$2.71 \cdot 10^{-3}$ (R; Ref. 6), $2.95 \cdot 10^{-3}$ (R; Ref. 8), $2.90 \cdot 10^{-3}$ (R; Ref. 14)	$3.1 \cdot 10^{-3}$
304.8		$3.81 \cdot 10^{-3}$ (T; Ref. 9)	$3.3 \cdot 10^{-3}$
305.3		$4.05 \cdot 10^{-3}$ (T; Ref. 9)	$3.3 \cdot 10^{-3}$
307.4		$4.38 \cdot 10^{-3}$ (T; Ref. 9)	$3.5 \cdot 10^{-3}$
308.2		$3.60 \cdot 10^{-3}$ (T; Ref. 14)	$3.6 \cdot 10^{-3}$
308.3		$4.56 \cdot 10^{-3}$ (T; Ref. 9)	$3.6 \cdot 10^{-3}$
309.8		$4.90 \cdot 10^{-3}$ (D; Ref. 9)	$3.8 \cdot 10^{-3}$
310.9	9.1 (Ref. 13)	$4.30 \cdot 10^{-3}$ (T; Ref. 13)	$3.9 \cdot 10^{-3}$
312.0		$5.38 \cdot 10^{-3}$ (D; Ref. 9)	$4.0 \cdot 10^{-3}$
313.2	136 (Ref. 6)	$3.66 \cdot 10^{-3}$ (T; Ref. 6)	$4.1 \cdot 10^{-3}$
314.7		$5.90 \cdot 10^{-3}$ (D; Ref. 9)	$4.3 \cdot 10^{-3}$
316.3		$6.27 \cdot 10^{-3}$ (D; Ref. 9)	$4.5 \cdot 10^{-3}$
320.4		$7.18 \cdot 10^{-3}$ (D; Ref. 9)	$5.1 \cdot 10^{-3}$
322.7		$7.62 \cdot 10^{-3}$ (D; Ref. 9)	$5.4 \cdot 10^{-3}$
323.2	136 (Ref. 6)	$4.57 \cdot 10^{-3}$ (T; Ref. 6)	$5.5 \cdot 10^{-3}$
333.2	136 (Ref. 6)	$5.73 \cdot 10^{-3}$ (T; Ref. 6)	$7.1 \cdot 10^{-3}$
343.2	136 (Ref. 6)	$8.30 \cdot 10^{-3}$ (T; Ref. 6)	$9.2 \cdot 10^{-3}$
353.2	136 (Ref. 6)	$1.07 \cdot 10^{-2}$ (T; Ref. 6)	$1.2 \cdot 10^{-2}$
363.2	170 (Ref. 6)	$1.54 \cdot 10^{-2}$ (T; Ref. 6)	$1.5 \cdot 10^{-2}$
367.6	111 (Ref. 13)	$1.86 \cdot 10^{-2}$ (T; Ref. 13)	$1.7 \cdot 10^{-2}$
373.2	204 (Ref. 6)	$2.02 \cdot 10^{-2}$ (T; Ref. 6)	$1.9 \cdot 10^{-2}$
423.4	627 (Ref. 13)	$5.96 \cdot 10^{-2}$ (T; Ref. 13)	$5.5 \cdot 10^{-2}$
479.5	2320 (Ref. 13)	$1.63 \cdot 10^{-1}$ (T; Ref. 13)	$1.6 \cdot 10^{-1}$
536.1	6500 (Ref. 13)	$4.08 \cdot 10^{-1}$ (T; Ref. 13)	$4.2 \cdot 10^{-1}$
550.4	8270 (Ref. 13)	$4.72 \cdot 10^{-1}$ (T; Ref. 13)	$5.2 \cdot 10^{-1}$
568.1	10680 (Ref. 13)	$6.91 \cdot 10^{-1}$ (T; Ref. 13)	$6.8 \cdot 10^{-1}$

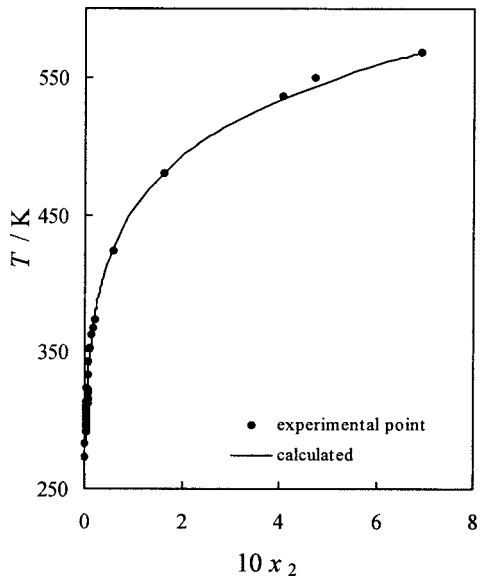

FIG. 5. All the solubility data for water (2) in ethylbenzene (1).

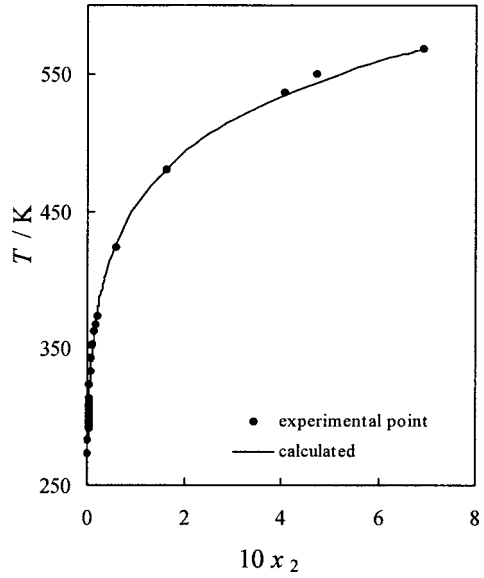

FIG. 6. Recommended and tentative solubility data for water (2) in ethylbenzene (1).

High Pressure Solubility of Ethylbenzene (1) in Water (2)

The experimental high pressure solubility for (1) in (2) investigated by Haruki *et al.*[12] at 553 and 583 K, and 10 400–26 400 kPa, and Sawamura *et al.*[30] at 273–323 K and 25 000–400 000 kPa have not been critically evaluated because the developed method is not applied for such data. An evaluation of these data was presented by Hefter and Young.[71]

Rejected and Inaccessible Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga[39] are independent data. The data reported by Alwani and Schneider,[35] Hicks and Young,[36] Roof,[37] and Scott and van Konynenburg,[38] lack sufficient information to justify evaluation. Therefore these data are Rejected.

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Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **72**, 5034 (1950).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

The solubility of ethylbenzene in water at 25 °C was reported to be 0.0168 $g(1)$/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is $2.85 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:
A mixture of (1) and (2) was rotated for 20 h in a constant temperature bath at 25 °C. A sample (5–20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10–50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

Source and Purity of Materials:
(1) Eastman Kodak Co. white label; fractionally distilled; b.p. 136.0 °C.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. Ben-Naim and J. Wilf, J. Phys. Chem. **70**, 771 (1979).

Variables:
Temperature: 10.0 and 20.0 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of ethylbenzene in water

t/°C	$10^3 \cdot$ mol(1)/L sln	$10^2 \cdot g(1)$/100 g sln (compilers)	$10^5 \cdot x_1$ (compilers)
10.0	1.91	2.03	3.44
20.0	2.00	2.13	3.61

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. A saturated solution was diluted several times and the optical density was measured by a Perkin-Elmer Model 450 spectrophotometer in the UV region of 200–400 nm.

Source and Purity of Materials:
(1) Fluka, puriss grade, purity ≥99.5%; used as received.
(2) Triply distilled.

Estimated Error:
Temperature: ±0.2 °C.
Solubility: 1% (reproducibility of measurements).

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. Ben-Naim and J. Wilf, J. Phys. Chem. **84**, 583 (1980).

Variables:
One temperature: 25.0 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of ethylbenzene in water

t/°C	mol (1)/L sln	$g(1)$/100 g sln (compilers)	x_1 (compilers)
25.0	$2.00 \cdot 10^{-3}$	$2.13 \cdot 10^{-2}$	$3.61 \cdot 10^{-5}$

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. Water (2) with an excess of ethylbenzene (1) was stirred for about 48 h in a thermostat and then the two phases were allowed to separate for about 24 h. Samples were analyzed spectroscopically in the UV region by a Perkin-Elmer model 450 spectrophotometer. Confirming results were obtained through contact between water and the vapor of the solute; the method was described in Ben-Naim *et al.*[1]

Source and Purity of Materials:
(1) Fluka, puriss grade, 99.9%; used as received.
(2) Triple distilled.

Estimated Error:
Temperature: ±0.2 °C.
Solubility: 1% (reproducibility of measurements).

References:
[1]A. Ben-Naim, J. Wilf, and M. Yaacobi, J. Phys. Chem. **77**, 95 (1973).

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. L. Bohon and W. F. Claussen, J. Am. Chem. Soc. **73, 1571 (1951).**

Variables:
Temperature: 0.4 °C–42.8 °C

Prepared By:
G. T. Hefter

Experimental Data

Solubility of ethylbenzene in water

t/°C	$10^5 \cdot x_1$ (compiler)	$g(1)$/100 g sln (compiler)[a]
0.4	3.71	0.0219
5.2	3.61	0.0213
20.7	3.51	0.0207
21.2	3.51	0.0207
25.0	3.53	0.0208[b]
25.6	3.54	0.0209
30.2	3.58	0.0211
34.9	3.75	0.0221
42.8	3.92	0.0231

[a]Solubilities of (1) in (2) were reported as ''optical density'' (absorbance) measurements. Solubilities were calculated by the compiler using the Beer-Lambert law, the stated cell path-length (1 cm) and the authors' ''extinction coefficients'' (absorptivities and corrected optical densities. This gave a solubility of $g(1)$/L sln which was then converted to $g(1)$/100 g sln by assuming a solution density of 1.00 kg/L.

[b]Given in the original paper as 0.208 $g(1)$/L.

Auxiliary Information

Method/Apparatus/Procedure:
A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24 h and then allowed to settle for at least another 24 h. Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been tarred, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of the samples were inserted into a quartz cuvette and measured in a Beckman DU spectrophotometer. Absorbances were corrected for adsorption of (1) onto the walls of the cuvette.

Source and Purity of Materials:
(1) Koppers Co., purified by redistillation, several washings, and passing through silica gel. Purity was determined by refractometry (no values given).
(2) Air-free conductivity water (no details given).

Estimated Error:
Temperature: ±0.02 °C.
Solubility: ±0.5% relative.

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. L. Brown and S. P. Wasik, J. Res. Natl. Bur. Stand., Sect. A **78**, 453 (1974).

Variables:
Temperature: 4.5°C–20.1 °C

Prepared By:
G. T. Hefter

Experimental Data

Solubility of ethylbenzene in water

t/°C	$10^5 \cdot x_1$ (compiler)	$g(1)$/100 g sln[a]
4.5	3.33	0.0196 ± 0.0004
6.3	3.26	0.0192 ± 0.0004
7.1	3.16	0.0186 ± 0.0006
9.0	3.18	0.0187 ± 0.0004
11.8	3.07	0.0181 ± 0.0005
12.1	3.11	0.0183 ± 0.0004
15.1	3.06	0.0180 ± 0.0005
17.9	3.12	0.0184 ± 0.0005
20.1	3.1	0.018 ± 0.0004[b]

[a]Errors given as standard deviations.

[b]Typographical error in original publication, digit missing in fourth decimal place.

Auxiliary Information

Method/Apparatus/Procedure:
Solubilities were calculated from partition coefficient measurements for the hydrocarbon between an aqueous solution and its vapor using headspace chromatography. The apparatus and the method of obtaining the partition coefficients are described in detail in the paper. Basically, the hydrocarbon was introduced as a vapor (to avoid emulsification) into a glass equilibration cell containing about 45 mL of water. The vapor was subsequently analyzed by gas chromatography using He as the carrier. Possible sources of error are discussed in detail although the source of vapor pressure data used to calculate solubilities is not given.

Source and Purity of Materials:
(1) 99.99 mole % purity; source and methods of purification not specified.
(2) Distilled.

Estimated Error:
Temperature: ± 0.01 °C.
Solubility: see table above.

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. Chen and J. Wagner, J. Chem. Eng. Data **39**, 679 (1994).

Variables:
Temperature: 303.15 K–373.15 K
Pressure: 1.36 bar, 2.04 bar

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of ethylbenzene in water

T/K	P/bar	$g(1)$/100 g sln (compilers)	$10^5 \cdot x_1$
303.15	1.36	0.0170	2.88 ± 0.04
313.15	1.36	0.0172	2.92 ± 0.04
323.15	1.36	0.0197	3.35 ± 0.09
333.15	1.36	0.0240	4.07 ± 0.23
343.15	1.36	0.0290	4.93 ± 0.21
353.15	1.36	0.0353	5.99 ± 0.24
363.15	1.70	0.0409	6.95 ± 0.17
373.15	2.04	0.0503	8.54 ± 0.34

Solubility of water in ethylbenzene

T/K	P/bar	$g(2)$/100 g sln (compilers)	$10^2 \cdot x_2$
303.15	1.36	0.0462	0.271 ± 0.018
313.15	1.36	0.0623	0.366 ± 0.023
323.15	1.36	0.0778	0.457 ± 0.025
333.15	1.36	0.0977	0.573 ± 0.026
343.15	1.36	0.1418	0.830 ± 0.066
353.15	1.36	0.1832	1.07 ± 0.047
363.15	1.70	0.2647	1.54 ± 0.134
373.15	2.04	0.3486	2.02 ± 0.064

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. A continuous flow equilibrium apparatus for mutual solubility measurements, Chen and Wagner,[1] was used. Samples were collected in 25 mL vials and 60 and 120 mL bottles containing anhydrous ethanol or dichloromethane as a solvent. Details of the standard preparation, calibration, and sampling procedures were described in Chen and Wagner.[2] A Hewlett-Packard 5880A gas chromatograph equipped with Porapac Q or GlasChrom 254 columns and a thermal conductivity detector was used for analysis. Reported solubilities are the average of 4–6 replicate determinations.

Source and Purity of Materials:
(1) Aldrich Chemical Co.; purity 99 mole %; used as received.
(2) Distilled and deionized water.

Estimated Error:
Temperature: ± 0.2 K.
Solubility: standard deviation as above.

References:
[1]H. Chen and J. Wagner, J. Chem. Eng. Data **39**, 470 (1994).
[2]H. Chen and J. Wagner, J. Chem. Eng. Data **39**, 475 (1994).

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
P. Dohanyosova, D. Fenclova, P. Vrbka, and V. Dohnal, J. Chem. Eng. Data **46**, 1533 (2001).

Variables:
Temperature: 273.65 K–328.15 K

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of ethylbenzene in water

T/K	$10^3 \cdot$ mol(1)/L sln	$10^2 \cdot g(1)$/100 g sln (compilers)	$10^5 \cdot x_1$
273.65	1.59	1.69	2.86
278.15	1.57	1.67	2.83
288.15	1.56	1.66	2.82
298.15	1.60	1.70	2.89
308.25	1.67	1.78	3.02
318.15	1.77	1.90	3.23
328.15	2.01	2.17	3.69

Auxiliary Information

Method/Apparatus/Procedure:
The solute vapor absorption method for preparation of the saturated solutions was used. Details of the apparatus, saturation procedure and sampling are described in the paper. The temperature was measured with a calibrated standard mercury thermometer to ±0.01 K. The samples were analyzed using a high performance liquid chromatograph (Ecom, Prague, Czech Republic) equipped with a Model LCP 4100 HPLC pump, a Model LCD 2082 UV detector, and a C18 glass analytical column. The analysis of each sample was replicated 6–10 times.

Source and Purity of Materials:
(1) Aldrich Chemical Co.; purity 99%, confirmed by liquid and gas chromatography, used as received.
(2) Distilled and treated by a Milli-Q water purification system.

Estimated Error:
Temperature: ±0.01 K.

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).

Variables:
Temperature: 10 °C–30 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

Solubility of water in ethylbenzene

t/°C	$10^3 \cdot x_2$ (compiler)	$g(2)$/100 g sln
10	1.62	0.0275
20	2.19	0.0373
30	2.95	0.0502

Auxiliary Information

Method/Apparatus/Procedure:
Component (1) was introduced into a thermostatted flask and saturated for 5 h with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

Source and Purity of Materials:
(1) Not specified.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
T. S. Filippov and A. A. Furman, Zh. Prikl. Khim. (Leningrad) **25**, 895 (1952).

Variables:
Temperature: 18.2 °C–49.5 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

Solubility of water in ethylbenzene

t/°C	$10^3 \cdot x_2$ (compiler)	$g(2)$/100 g sln
18.2	1.74	0.0296
18.3	1.81	0.0308
19.7	1.92	0.0327
22.3	2.07	0.0352
23.4	2.12	0.0360
24.2	2.28	0.0388
27.2	2.91	0.0494
29.8	3.50	0.0595
31.6	3.81	0.0648
32.1	4.05	0.0679
34.2	4.38	0.0745
35.1	4.56	0.0777
36.6	4.90	0.0835
38.8	5.38	0.0917
41.5	5.90	0.1005
43.1	6.27	0.1070
47.2	7.18	0.1225
49.5	7.62	0.13000

Auxiliary Information

Method/Apparatus/Procedure:
Weighed amounts of both components were placed in glass tubes, 40 mm across and 65 mm long, and shaken. Clear and cloud points were observed 5–6 times to within 0.2 °C–0.3 °C.

Source and Purity of Materials:
(1) Source not specified; distilled; no turbidity if cooled to − 10 or − 20 °C.
(2) Twice distilled.

Estimated Error:
Temperature: ± 0.3 °C.
Solubility: not specified.

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. Fühner, Ber. Dtsch. Chem. Ges. **57**, 510 (1924).

Variables:
One temperature: 15 °C

Prepared By:
A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Data

The solubility of ethylbenzene in water at 15 °C was reported to be 0.014 $g(1)$/100 g sln.

The corresponding mole fraction, x_1 , calculated by the compilers is $2.4 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:
In a stoppered volumetric cylinder, pipetted volumes or weighed amounts of (1) were added with shaking to 50, 100, or 1000 mL (2) until a completely clear solution was no longer obtained at the experimental temperature.

Source and Purity of Materials:
(1) Source not specified; commercial grade; used as received.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. N. Guseva and E. I. Parnov, Zh. Fiz. Khim. **38**, 805 (1964).

Variables:
Temperature: 115.0 °C–233.5 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

Solubility of ethylbenzene in water

t/°C	$10^4 \cdot x_1$ (compiler)	$g(1)$/100 g sln
115.0	0.871	0.0513
140.5	2.02	0.119
170.5	6.04	0.355
210.0	11.27	0.661
233.5	19.33	1.129

Auxiliary Information

Method/Apparatus/Procedure:
The measurements were made in sealed glass tubes. No details were reported in the paper.

Source and Purity of Materials:
(1) Not specified.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
M. Haruki, Y. Iwai, S. Nagao, and Y. Arai, J. Chem. Eng. Data **46**, 950 (2001).

Variables:
Temperature: 573.2 K and 583.2 K
Pressure: 10.4 MPa–26.4 MPa

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Mutual solubility of ethylbenzene in water

T/K	P/MPa	$g(1)$/100 g sln (compilers)	x_1
573.2	10.4	0.034	0.006 ± 0.0012
	14.4	0.034	0.006 ± 0.0012
	17.5	0.040	0.007 ± 0.0010
	20.4	0.040	0.007 ± 0.0009
	23.4	0.040	0.007 ± 0.0014
	26.4	0.040	0.007 ± 0.0009
583.2	17.1	0.117	0.022 ± 0.0020
	20.5	0.122	0.021 ± 0.0016
	23.4	0.122	0.021 ± 0.0011
	26.3	0.107	0.020 ± 0.0010

Mutual solubility of water in ethylbenzene

T/K	P/MPa	$g(2)$/100 g sln (compilers)	x_2
573.2	10.4	15.6	0.521 ± 0.0149
	14.4	15.0	0.508 ± 0.0117
	17.5	14.4	0.498 ± 0.0162
	20.4	13.0	0.469 ± 0.0241
	23.4	12.8	0.463 ± 0.0119
	26.4	12.3	0.453 ± 0.0198
583.2	12.6	41.8	0.809 ± 0.0080
	14.5	33.3	0.746 ± 0.0057
	17.1	30.3	0.719 ± 0.0076
	20.5	28.4	0.700 ± 0.0086
	23.4	26.5	0.680 ± 0.0034
	26.3	25.1	0.664 ± 0.0146

Auxiliary Information

Method/Apparatus/Procedure:
A flow-type apparatus to measure the phase equilibria at high temperatures and pressures was used, details were described in Haruki *et al.*[1] Pressure was controlled by back-pressure-regulators. The phase behavior was observed with a video camera attached to a telescope. Samples of each phase were collected in bottles containing ethanol to obtain homogenous solutions. The compositions of samples were analyzed by a gas chromatograph with a thermal conductivity detector. Solubilities reported above are the arithmetic average of 8–18 experimental points.

Source and Purity of Materials:
(1) Wako Pure Chem. Ind.; purity >98mole % by glc; used as received.
(2) Distilled water was purified by Milliq-Labo (Millipore Co.) equipment.

Estimated Error:
Temperature: ± 1 K.
Pressure: ± 0.1 MPa.

References:
[1]M. Haruki, Y. Iwai, S. Nagao, Y. Yahiro, and Y. Arai, J. Chem. Eng. Res. **39**, 4516 (2000).

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. L. Heidman, C. Tsonopoulos, C. J. Brady, and G. M. Wilson, AIChE J. **31**, 376 (1985).

Variables:
Temperature: 311 K–568 K
Pressure: 0.01 MPa–10.7 MPa

Prepared By:
G. T. Hefter

Experimental Data

Solubility of ethylbenzene in water

T/K	$10^4 \cdot x_1$	$g(1)$/100 g sln (compiler)	P/MPa
311.5	0.32	0.019	not specified
367.6	0.86	0.051	0.111
423.4	2.19	0.129	0.627
479.5	6.0	0.35	2.32
536.1	32.5	1.88	6.50
552.8	37.5	2.17	8.59

Solubility of water in ethylbenzene

T/K	$10^2 \cdot x_2$	$g(2)$/100 g sln (compiler)	P/MPa
310.9	0.43	0.073	0.0091[a]
367.6	1.86	0.320	0.111
423.4	5.96	1.06	0.627
479.5	16.3	3.20	2.32
536.1	40.8	10.5	6.50
550.4	47.2	13.2	8.27
568.1[b]	69.1[b]	27.5	10.68[b]

[a]Estimated by the authors from pure component data.

[b]Three phase critical point.

The three phase critical point was reported to be 568.1±0.6 K, 10.68±0.04 MPa, and $x_1 = 5.83 \cdot 10^{-3}$ [3.34 $g(1)$/100 g sln, compiler].

The authors also report an equation providing a fit of their own and literature data over the range 273 K–568 K, viz.

$$\ln x_1 = -185.1695 + 7348.55/T + 26.34525 \ln T$$

$$\ln x_2 = -0.37215 - 4.4626(T_r^{-1} - 1) - 0.38596(1 - T_r)^{1/3} - 2.59850(1 - T_r)$$

where T_r=T/568.1

Auxiliary Information

Method/Apparatus/Procedure:
Experimental procedure was similar to that used in Ref. 1. Hydrocarbons were determined by gas chromatography and water by the Karl Fischer titration. Critical points were determined by the synthetic method using visual observation. This aspect of the procedure is discussed in detail in the paper.

Source and Purity of Materials:
(1) Aldrich 99+ mol %; water free purity greater or equal to 99.9 mol %, checked by gas chromatography.
(2) Distilled; no details given.

Estimated Error:
Temperature: not stated.
Solubility: ±5%, relative precision of replicate analyses.
Pressure ±1%; type of error not stated.

References:
[1]C. Tsonopoulos and G. M. Wilson, AIChE J. **29**, 990 (1983).

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. R. Jones and C. B. Monk, J. Chem. Soc. 2633 (1963).

Variables:
Temperature: 25 °C–35 °C

Prepared By:
A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Data

Solubility of water in ethylbenzene

t/°C	$10^4 \cdot$ mL(2)/mL(1)
25	3.7
30	4.3
35	5.3

Auxiliary Information

Method/Apparatus/Procedure:
In a thermostatted glass stoppered flask 10–25 mL(1) was shaken for a minimum of 4 h with tritiated water (a few mL of HTO equivalent to ~2 mci/mL) and decanted. A 5 mL aliquot was reshaken for 4 h with 5 mL H_2O in a 10 mL flask, sampled and assayed with a Nuclear Enterprises type 8301 liquid scintillation counter. The two-stage process eliminates quencing effects (due to solvent) on the scintillator.

Source and Purity of Materials:
(1) Laboratory grade; dried over $CaCl_2$ and fractionally distilled.
(2) Not specified.

Estimated Error:
Solubility: ±5% to ±1% (average deviation).

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
D. F. Keeley, M. A. Hoffpauir, and J. R. Meriwether, J. Chem. Eng. Data **36**, 456 (1991).

Variables:
One temperature: 298.15 K

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of ethylbenzene in water

T/K	mol (1)/L sln	$g(1)$/100 g sln (compilers)	x_1 (compilers)
298.15	$(1.66 \pm 0.04) \cdot 10^{-3}$	$1.77 \cdot 10^{-2}$	$3.00 \cdot 10^{-5}$

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was determined by a headspace chromatographic analysis, Ref. 1, using a multiple injection interrupted flow technique. Samples were prepared in septum bottles of 160 mL volume which were thermostatted and shaken for 72 h prior to analysis. For analysis each bottle was transferred to a tempering beaker and pressurized to 15.00 psig with chromatographic grade nitrogen. Bottles were attached to the headspace sampling port of a chromatograph with 1 m by 3.2 mm stainless steel column (5% SP-1200, 1.75% Bentone-34) on 100/1200 mesh Supelcoport (Supelco Inc.) and FID detector. Solubility was calculated on the basis of Henry's law.

Source and Purity of Materials:
(1)Baker, fractionally distilled, purity 99.40% by glc.
(2) Deionized water.

Estimated Error:
Temperature: ± 0.05 K.

References:
[1]D. F. Keeley and J. R. Meriwether, Rev. Sci. Instrum. **57**, 1434 (1986)

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. B. Klevens, J. Phys. Chem. **54**, 283 (1950).

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

The solubility of ethylbenzene in water at 25 °C was reported to be 0.175 $g(1)$/L sln and $1.64 \cdot 10^{-3}$ mol(1)/L sln.
The corresponding mass percent and mole fraction calculated by the compiler are 0.0175 $g(1)$/100 g sln and $x_1 = 2.9 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 L of (2) for as long as 3 months. Aliquots were removed and concentrations determined by spectra.

Source and Purity of Materials:
(1) Not specified.
(2) Not specified.

Estimated Error:
Not specified.

Components:	Original Measurements:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4] (2) Water; H_2O; [7732-18-5]	I. M. Korenman and R. P. Aref'eva, Patent USSR, 553 524, 1977.04.05.
Variables:	**Prepared By:**
One temperature: 20 °C	A. Maczynski

Experimental Data

The solubility of ethylbenzene in water at 20 °C was reported to be 0.21 $g(1)$/L(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.021 $g(1)$/100 g sln and $3.6 \cdot 10^{-5}$. The assumption that 1 L sln=1 kg sln was used in the calculation.

Auxiliary Information

Method/Apparatus/Procedure:

About 100–500 mL (2) was placed in a glass cylinder and 10–50 mg of an insoluble indicator was added and (1) was microburetted until the indicator floated to form a colored thin layer on the cylinder wall 2–3 mL above the liquid layer. After each drop of (1), the mixture was vigorously mixed for 0.5–1.5 min.

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:

Not specified.

Components:	Original Measurements:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4] (2) Water; H_2O; [7732-18-5]	I. M. Korenman and R. P. Aref'eva, Zh. Prikl. Khim. (Leningrad) **51**, 957 (1978).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and Z. Maczynska

Experimental values

The solubility of ethylbenzene in water at 25 °C was reported to be 0.18 $g(1)$/L sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.018 $g(1)$/100 g sln and $3.1 \cdot 10^{-5}$. The assumption that 1.00 L sln=1.00 kg sln was used in the calculation.

Auxiliary Information

Method/Apparatus/Procedure:

About 200–500 mL (2) was placed in a ground-joint glass cylinder and 20–50 mg of an insoluble indicator (dithizon, phenolphthalein, etc.) was added, and (1) was microburetted until the indicator floated to form a colored thin layer on the cylinder wall above the liquid layer. Blanks were made to determine the excess of (1).

Source and Purity of Materials:

(1) Not specified.
(2) Not specified.

Estimated Error:

Solubility: 0.01 $g(1)$/L sln (standard deviation from 6 determinations).

Components:	Original Measurements:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4] (2) Water; H_2O; [7732-18-5]	C. McAuliffe, Nature (London) **200**, 1092 (1963).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and Z. Maczynska

Experimental Data

The solubility of ethylbenzene in water at 25 °C was reported to be 0.0159 $g(1)$/100 g sln.

The corresponding mole fraction, x_1 , calculated by the compilers is $2.70 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:

The saturated solution of (1) in (2) was prepared by either shaking vigorously on a reciprocal shaker or stirring for several days with a magnetic stirrer. A 0.05 mL or 0.10 mL sample of the hydrocarbon-saturated water was injected directly into a gas liquid chromatograph.

Source and Purity of Materials:

(1) Phillips Petroleum Co.; 99+%; used as received.
(2) Distilled.

Estimated Error:

Temperature: ± 1.5 °C.
Solubility: 0.0008 (standard deviation of mean).

Components:	Original Measurements:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4] (2) Water; H_2O; [7732-18-5]	C. McAuliffe, J. Phys. Chem. **70**, 1267 (1966).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski, Z. Maczynska, and A. Szafranski

Experimental Data

The solubility of ethylbenzene in water at 25 °C was reported to be 152 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are $0.0152g(1)$/100 g sln and $2.57 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:

In a 250 mL bottle, 10–20 mL of (1) was vigorously shaken for 1 h, or magnetically stirred for 1 day, with 200 mL of (2) at 25 °C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.

Source and Purity of Materials:

(1) Phillips Petroleum or Columbia Chemical; used as received.
(2) Distilled.

Estimated Error:

Temperature: ± .5 °C.
Solubility: 8 mg (1)/kg (2) (standard deviation of mean).

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
T. J. Morrison and F. Billett, J. Chem. Soc. 3819 (1952).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski

Experimental Data

The solubility of ethylbenzene in water at 25 °C was reported to be $1.55 \cdot 10^{-3}$ mol (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by compilers are 0.0165 $g(1)$/100 g sln and $x_1 = 2.8 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:

After an excess of (1) was shaken with about 1 L of (2) for about 1 week, a known volume of saturated solution was made slightly alkaline, and a stream of pure air passed through to drive off the (1). After passage through a silica tube packed with cupric oxide and heated to redness, the (2) was removed by concentrated sulfuric acid and calcium chloride and the carbon dioxide absorbed and weighed in soda-asbestos. The precautions usual in organic combustions were taken.

Source and Purity of Materials:

(1) Source not specified; purest obtainable material; distilled; purity not specified.
(2) Not specified.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: ±1% (mean of large numbers of determinations).

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. W. Owens, S. P. Wasik, and H. DeVoe, J. Chem. Eng. Data **31**, 47 (1986).

Variables:
Temperature: 10.0 °C–45.0 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of ethylbenzene in water

t/°C	$10^3 \cdot$ mol (1)/L sln	$g(1)$/100 g sln (compilers)	$10^5 \cdot x_1$ (compilers)
10.0	1.850±0.084	0.01964	3.334
14.0	1.812±0.050	0.01925	3.267
17.0	1.776±0.061	0.01887	3.203
18.0	1.725±0.013	0.01834	3.112
19.0	1.676±0.064	0.01782	3.024
20.0	1.770±0.032	0.01882	3.194
21.0	1.724±0.030	0.01834	3.112
22.0	1.713±0.072	0.01822	3.093
24.0	1.751±0.088	0.01864	3.163
25.0	1.811±0.028	0.01928	3.272
26.0	1.753±0.037	0.01867	3.168
28.0	1.747±0.038	0.01861	3.159
30.0	1.777±0.103	0.01894	3.215
35.0	1.818±0.051	0.01941	3.295
40.0	1.928±0.060	0.02063	3.500
45.0	1.991±0.053	0.02134	3.622

Auxiliary Information

Method/Apparatus/Procedure:

The solubilities were determined by the technique reported in May *et al.*[1] and DeVoe *et al.*[2] using an automated coupled-column liquid chromatographic apparatus, described in Owens *et al.*[3] A saturated solution was generated by pumping water through a column containing the solute coated on Chromosorb W. A known volume of the saturated solution was passed through a small extractor column filled with reverse phase packing where the solute was removed quantitatively. The extracted solute was then eluted with a water-methanol mixture, separated from impurities on an HPLC analytical column, and analyzed by UV spectrophotometry at 254 nm. The standard deviation of the peak area for the known solution was <2.4%. 3–10 measurements at each temperature were made.

Source and Purity of Materials:

(1) Aldrich Chemical Co.; used as received; purity >99% by glc.
(2) HPCL grade.

Estimated Error:

Temperature: ±0.05 °C.
Solubility: as above.

References:

[1]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).
[2]H. DeVoe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. (USA) **86**, 361 (1981).
[3]J. W. Owens, T. J. Buckley, and H. DeVoe, J. Res. Natl. Bur. Stand. (USA) **90**, 41 (1985).

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. Polak and B. C.-Y. Lu, Can. J. Chem. **51**, 4018 (1973).

Variables:
Temperature: 0 °C–25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

Solubility of ethylbenzene in water

t/°C	$10^5 \cdot x_1$ (compiler)	g (1)/100 g sln (compiler)	mg (1)/kg (2)
0[a]	3.34	0.0197	197[c]
25[b]	3.00	0.0177	177[c]

Solubility of water in ethylbenzene

t/°C	$10^3 \cdot x_2$ (compiler)	g (2)/100 g sln (compiler)	mg (2)/kg (1)
0[a]	1.05	0.0178	178[d]
25[b]	2.60	0.0442	442[c]

[a–e]See Estimated Error.

Auxiliary Information

Method/Apparatus/Procedure:
Approximately 50 mL of (1) together with (2) were placed in a 125 mL Hypo-vial which was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 h and left in the bath for 3 days or was kept in the bath without stirring for 7 days, before samples were taken for analysis.

The solubility of water in the organic layer was determined by the Karl Fischer titration and the solubility of hydrocarbon in the water layer was determined by gas chromatography.

Source and Purity of Materials:
(1) Phillips Petroleum Co.; pure grade reagent 99+%; shaken three times with distilled water.
(2) Distilled.

Estimated Error:
Temperature: (a) ±0.02 °C, (b) ±0.01 °C.
Solubility: (c) ±1.7%, (d) ±4.7%, (e) ±3.1% (from two or three determinations)

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

The solubility of ethylbenzene in water at 25 °C and at system pressure was reported to be 131.0 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are $0.0131g(1)/100$ g sln and $2.22 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and ensured saturation of the (2) phase in 2–4 days. Analyses were carried out by glc using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

Source and Purity of Materials:
(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.
(2) Distilled.

Estimated Error:
Temperature: ±1 °C.
Solubility: ±1.4 mg(1)/kg(2).

Components:	**Original Measurements:**
(1) Ethylbenzene; C_8H_{10} ; [100-41-4] (2) Water; H_2O; [7732-18-5]	I. Sanemasa, S. Arakawa, M. Araki, and T. Deguchi, Bull. Chem. Soc. Jpn. **57**, 1539 (1984).
Variables:	**Prepared By:**
One temperature: 25 °C	G. T. Hefter

Experimental Data

The solubility of ethylbenzene in water at 25 °C was reported to be $1.62 \cdot 10^{-3}$ mol(1)/L sln.

Assuming a solution density of 1.00 kg/L this corresponds to a solubility of 0.0172 $g(1)$/100 g sln, $x_1 = 2.92 \cdot 10^{-5}$, calculated by the compiler.

Auxiliary Information

Method/Apparatus/Procedure:

The apparatus used is described in detail in Sanemasa *et al.*[1] The method involves the introduction of solute vapor (1) into liquid (2) by bubbling air through liquid (1) using a recirculating pump in a closed system. After solubility equilibrium was attained an aliquot of the saturated aqueous solution was withdrawn and analyzed by solvent extraction-UV spectrophotometry.

Source and Purity of Materials:

(1) Analytical reagent grade, source and purity not stated, used without further purification.
(2) Deionized and redistilled; no further details given.

Estimated Error:

Not specified.

References:

[1]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).

Components:	**Original Measurements:**
(1) Ethylbenzene; C_8H_{10} ; [100-41-4] (2) Water; H_2O; [7732-18-5]	I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Chem. Lett. 225 (1981).
Variables:	**Prepared By:**
Temperature: 15 °C–45 °C	M. C. Haulait-Pirson

Experimental Data

Solubility of ethylbenzene in water

t/°C	$10^4 \cdot x_1$[a]	$g(1)$/100 g sln[a]	$g(1)$/L sln
15	2.99	0.0176	0.176 ± 0.009
25	3.09	0.0182	0.181 ± 0.006
35	3.31	0.0195	0.194 ± 0.006
45	3.69	0.0217	0.215 ± 0.004

[a]Assuming the solution density to be that of pure water at the same temperature.[1]

Auxiliary Information

Method/Apparatus/Procedure:

The apparatus used for attaining solubility equilibrium is described in detail in the paper. Liquid (1) and redistilled (2) were placed in a vessel and a thermostatted funnel, respectively. The solute vapor, generated by bubbling air through the liquid solute, was introduced into the funnel and circulated by means of a pump. The circulation rate was 2 L/min. Solubility equilibria were attained within 5 min. Then portions of 10 mL of the aqueous sln were transferred to funnels to which 10 mL of chloroform had been added. Experimental procedures involved in spectrophotometric measuring the chloroform extracts were not reported. The solubility runs were made such that the temperature of solute reservoir was made to vary while that of solvent phase was held constant. The solubility obeys Henry's law at constant solvent temperature. Solubility values were calculated from Henry's law constants.

Source and Purity of Materials:

(1) Analytical reagent grade used as purchased.
(2) Redistilled.

Estimated Error:

Solubility: given above.

References:

[1]*CRC Handbook of Chemistry and Physics*, R.C. Weast, Editor, 63rd ed. (CRC, Boca Raton, FL, 1982).

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).

Variables:
Temperature: 15 °C-45 °C

Prepared By:
G. T. Hefter

Experimental Data

Solubility of ethylbenzene in water

t/°C	$10^5 \cdot x_1$ (compiler)[a]	$g(1)$/100 g sln (compiler)[a]	$10^3 \cdot$ mol(1)/L sln
15	2.72	0.0160	1.51 ± 0.08
25	2.87	0.0169	1.59 ± 0.05
35	2.99	0.0176	1.54 ± 0.05
45	3.33	0.0196	1.83 ± 0.05

[a]Assuming solution densities to be the same as those of pure water at the same temperature (Kell[1]).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to an earlier design (Sanemasa *et al.*[2]) and is described in detail in the paper. 100–200 mL of (2) and 10–20 mL of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was established a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 mL aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.

Source and Purity of Materials:
(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 98.0%, used without further purification.
(2) Redistilled; no further details given.

Estimated Error:
Temperature: ±0.01 °C.
Solubility: see table, type of error not specified.

References:
[1]G. S. Kell, J. Chem. Eng. Data **20**, 97 (1975).
[2]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Chem. Lett. 225 (1981).

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. Sanemasa, Y. Miyazaki, S. Arakawa, M. Kumamaru, and T. Deguchi, Bull. Chem. Soc. Jpn. **60**, 517 (1987).

Variables:
One temperature: 25.0 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of ethylbenzene in water

t/°C	mol (1)/L sln	$g(1)$/100 g sln (compilers)	x_1 (compilers)
25.0	$1.37 \cdot 10^{-3}$	$1.46 \cdot 10^{-2}$	$2.48 \cdot 10^{-5}$

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. The apparatus used for preparing aqueous solutions saturated with hydrocarbon vapor was the same as that previously reported in Sanemasa *et al.*[1] The method was based on the introduction of phase (1) (by bubbling air through the mixture using circulating pump in a closed system) into 100 mL of water. After 10 min (at circulation rate of vapor of 1.5 L/min) equilibrium was attained, and a 30 mL portion of the saturated aqueous solution was transferred into three separatory funnels with 5 mL of toluene. Mixtures were analyzed by gas chromatography.

Source and Purity of Materials:
(1) Source not specified; analytical reagent grade; purity 98%; used as received.
(2) Deionized and redistilled.

Estimated Error:
Temperature: ±0.1 °C

References:
[1]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
S. Sawamura, K. Nagaoka, and T. Machikawa, J. Phys. Chem. B **105**, 2429 (2001).

Variables:
Temperature: 273.2 K–323.2 K
Pressure: 0.1 MPa–400 MPa

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of ethylbenzene in water

T/K	P/MPa	$g(1)$/100 g sln (compilers)	$10^5 \cdot x_1$
273.2	0.1	0.01906	3.234
278.2	0.1	0.01817	3.084
283.2	0.1	0.01746	2.964
288.2	0.1	0.01697	2.880
293.2	0.1	0.01687	2.863
298.2	0.1	0.01697	2.880
303.2	0.1	0.01736	2.946
308.2	0.1	0.01795	3.047
313.2	0.1	0.01878	3.188
318.2	0.1	0.01967	3.338
323.2	0.1	0.02077	3.525
273.2	25	0.01962	3.329
298.2	25	0.01760	2.987
313.2	25	0.01989	3.375
273.2	50	0.02055	3.488
283.2	50	0.01934	3.283
298.2	50	0.01894	3.214
313.2	50	0.02067	3.508
323.2	50	0.02241	3.804
273.2	75	0.02099	3.563
313.2	75	0.02126	3.609
273.2	100	0.02131	3.617
283.2	100	0.02006	3.404
298.2	100	0.01952	3.312
313.2	100	0.02165	3.675
323.2	100	0.02330	3.954
273.2	150	0.02116	3.591
283.2	150	0.01994	3.384
298.2	150	0.01972	3.347
313.2	150	0.02204	3.741
323.2	150	0.02474	4.199
273.2	200	0.01979	3.358
283.2	200	0.01944	3.300
298.2	200	0.01943	3.298
313.2	200	0.02214	3.758
323.2	200	0.02524	4.283
273.2	250	0.01857	3.151
283.2	250	0.01857	3.151
298.2	250	0.01894	3.214
313.2	250	0.02182	3.704
323.2	250	0.02528	4.291
273.2	300	0.01746	2.964
283.2	300	0.01785	3.030
298.2	300	0.01821	3.090
313.2	300	0.02143	3.637
323.2	300	0.02474	4.199
273.2	350	0.01636	2.776
283.2	350	0.01687	2.863
298.2	350	0.01739	2.952
313.2	350	0.02077	3.525
323.2	350	0.02403	4.078
273.2	400	0.01537	2.609
283.2	400	0.01609	2.730
298.2	400	0.01631	2.768
313.2	400	0.02006	3.404
323.2	400	0.02281	3.871

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. Water and a few drops of ethylbenzene were placed in a high pressure optical cell with a Teflon ball for stirring as described in Sawamura *et al.*[1] The sample was pressurized and shaken in a thermoregutated water bath for a few days. The absorbance was measured at the absorption maximum around 260 nm. Details of the apparatus, procedures, and purification were reported in Refs. 1 and 2. Solubilities were calculated on the basis of measurements and recommended solubility value at 298.15 K and 0.1 MPa reported in Shaw.[3]

Source and Purity of Materials:
(1) Nacalai Tesque, Co.; shaken successively with H_2SO_4, Na_2CO_3 aq, H_2O, dried over $MgSO_4$, distilled; Sawamura *et al.*[2]
(2) Deionized; distilled over trace of $KMnO_4$, Sawamura *et al.*[2]

Estimated Error:
Temperature: ± 0.1 K (compilers).

References:
[1]S. Sawamura, K. Suzuki, and Y. Taniguchi, J. Sol. Chem. **16**, 649 (1987).
[2]S. Sawamura, K. Kitamura, and Y. Taniguchi, J. Phys. Chem. **93**, 4931 (1989).
[3]D. G. Shaw, (ed.), *IUPAC Solubility Data Series*, Vol. 37 (Pergamon, New York, 1989).

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
S. Sawamura, K. Kitamura, and Y. Taniguchi, J. Phys. Chem. **93**, 4931 (1989).

Variables:
Temperature: 25.00 °C
Pressure: 0.1MPa –400 MPa

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of ethylbenzene in water

t/°C	P/MPa	mol (1)/L sln	x_p/x_0	$10^4 \cdot g(1)$/100 g sln (compilers)	$10^5 x_1$ (compilers)
25.00	0.1	$1.8 \cdot 10^{-3}$	1	1.92	3.25
	25		1.037	1.99	3.37
	50		1.116	2.14	3.63
	100		1.150	2.20	3.74
	150		1.162	2.23	3.78
	200		1.145	2.19	3.72
	250		1.116	2.14	3.63
	300		1.073	2.06	3.49
	350		1.025	1.96	3.33
	400		0.961	1.84	3.13

x_p/x_0=relation of solubilities at high and normal pressure.

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. Water and a few drops of ethylbenzene were placed in a high pressure optical cell with a Teflon ball for stirring as described in Sawamura *et al.*[1] The sample was pressurized and shaken in a thermoregutated water bath for 5 h. The absorbance was measured with a Hitachi Model 340 double-beam spectrophotometer. Details of the apparatus, procedures, and purification were reported in Sawamura *et al.*[1] Solubilities were calculated through the Lambert-Beer's law with use of the molar extinction coefficients. The ratios of solubilities at high and atmospheric pressures are the average of at least 3 measurements.

Source and Purity of Materials:
(1) Nacalai Tesque, Co.; shaken successively with H_2SO_4, Na_2CO_3 aq, H_2O, dried over $MgSO_4$, distilled.
(2) Not specified.

Estimated Error:
Temperature: ±0.01 °C.

References:
[1]S. Sawamura, K. Suzuki, and Y. Taniguchi, J. Sol. Chem. **16**, 649 (1987).

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
F. P. Schwarz and J. Miller, Anal. Chem. **52**, 2162 (1980).

Variables:
Temperature: 10.0 °C–30.0 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of ethylbenzene in water

t/°C	$g(1)$/100 g sln	$10^5 \cdot x_1$ (compilers)
10.0[a]	0.0211±0.0003	3.58
10.0[b]	0.0180±0.0014	3.05
20.0[a]	0.0208±0.0011	3.53
20.0[b]	0.0184±0.0013	3.12

Auxiliary Information

Method/Apparatus/Procedure:
Two methods, (a) the elution chromatography method, described in Schwarz,[1] and (b) the UV absorption method were used. For (a) the 3 mm o.d. columns ~25 cm long and containing 0.3–0.5 g of (1) were used. The measurement time was 1–14 days. Each solubility was determined from 2 different columns. For (b) a solution obtained in an equilibrium apparatus was diluted with ethanol, UV absorption measurements were performed and compared with solutions of known composition. Each solubility was determined twice. Details of the apparatus and procedures were described in the paper.

Source and Purity of Materials:
(1) Source not specified, reagent grade material.
(2) Distilled water

Estimated Error:
Temperature: ±0.5 °C
Solubility: as above.

References:
[1]F. P. Schwarz, Anal. Chem. **52**, 10 (1980).

Components:	**Original Measurements:**
(1) Ethylbenzene; C_8H_{10} ; [100-41-4] (2) Water; H_2O; [7732-18-5]	C. Sutton and J. A. Calder, J. Chem. Eng. Data, **20**, 320 (1975).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and Z. Maczynska

Experimental Data

The solubility of ethylbenzene in water at 25 °C was reported to be 161.2 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.01612 $g(1)$/100 g sln and $2.734 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:

The concentration of (1) in (2) was determined by gas chromatography.

Source and Purity of Materials:

(1) Aldrich Chemical Co. or Matheson, Coleman, and Bell 99+%.
(2) Distilled.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: 0.9 mg (1)/kg (2) (standard deviation of the mean for six replicates).

Components:	**Original Measurements:**
(1) Ethylbenzene; C_8H_{10} ; [100-41-4] (2) Water; H_2O; [7732-18-5]	Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of ethylbenzene in water

t/°C	mol (1)/L sln	g (1)/100 g sln (compilers)	x_1 (compilers)
25.0	$1.76 \cdot 10^{-3}$	$1.874 \cdot 10^{-2}$	$3.18 \cdot 10^{-5}$

Auxiliary Information

Method/Apparatus/Procedure:

A generator column method was used as described in DeVoe *et al.*[1] and May *et al.*[2] A column was coated with (1) by pulling about 2 mL of liquid through the clean dry support (Chromosorb W-HP). A saturated solution was generated by pumping water into the inlet of the coated column and was then analyzed by hplc. The column was thermostatted by pumping water from a bath through a column jacket. An average of at least three measurements is reported.

Source and Purity of Materials:

(1) Source not specified; purity >99 mole % checked by high temperature glc.
(2) Source not specified.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: 1% (estimated by the authors).

References:

[1]H. De Voe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. (USA) **86**, 361 (1981).
[2]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).

Components:
(1) Ethylbenzene; C_8H_{10} ; [100-41-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. Vesala, Acta Chem. Scand., Ser. A **28**, 839 (1974).

Variables:
One temperature: 298.15 K

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of ethylbenzene in water

T/K	mol (1)/g (2)	$g(1)$/100 g sln (compilers)	x_1 (compilers)
298.15	$(1.91\pm0.02)\cdot10^{-6}$	$2.03\cdot10^{-4}$	$3.44\cdot10^{-5}$

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. The equilibration was carried out in a modified vessel, Franks *et al.*,[1] equipped with a magnetic stirrer. The temperature of the water bath was maintained within ±0.05 K. Equilibrium was obtained after 48 h and then samples were analyzed by spectrophotometry. At least 5 parallel determinations were performed.

Source and Purity of Materials:
(1) Commercial analytical grade reagent; purity 99% by glc; distilled through a column.
(2) Distilled water passed through an Amberlite CG 120+CG 400 ion-exchange column.

Estimated Error:
Temperature: ±0.05 K.
Solubility: as above.

References:
[1]F. Franks, M. Gent, and H. H. Johnson, J. Chem. Soc. 2716 (1963).

2.3. *o*-Xylene+Water

Components:
(1) *o*-Xylene (1,2-dimethylbenzene); C_8H_{10} ; [95-47-6]
(2) Water; H_2O; [7732-18-5]

Evaluators:
A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, January, 2004.

Critical Evaluation of the Solubility of *o*-Xylene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below:

Author (s)	T/K	Author (s)	T/K
Andrews and Keefer[1]	298	Price[8]	298
Ben-Naim and Wilf[2]	283–293	Sanemasa *et al.*[9]	288–318
Guseva and Parnov[3]	412–524	Sanemasa *et al.*[10]	298
Keeley *et al.*[5]	298	Sawamura *et al.*[11]	298
McAuliffe[6]	298	Sutton and Calder[12]	298
Polak and Lu[7]	273 and 298	Tewari *et al.*[13]	298

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 2 and expressed by the equation:

$$\ln x_1 = \ln x_{\min,1} + D[(T_{\min}/T)\ln(T_{\min}/T) + 1 - (T_{\min}/T)], \quad (1)$$

where $\ln x_{\min,1} = -10.26$, $D = 40.4$, and $T_{\min} = 290$.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the Reference data. Comparison between Reference and experimental data is one of the criteria used to assign data to the categories listed in Table 7.

TABLE 7. The data categories for solubility of *o*-xylene (1) in water (2)

T/K	Recommended [data in good agreement (±30%) with each other and with the reference data]	Tentative [data in good agreement (±30%) with the reference data]	Doubtful [data in poor agreement (>30%) with the reference data]
273.2			Polak and Lu[7]
283.2		Ben-Naim and Wilf[2]	
288.2		Sanemasa *et al.*[9]	
293.2		Ben-Naim and Wilf[2]	
298.1		Sanemasa *et al.*[10]	
298.2	Andrews and Keefer[1] Keeley *et al.*[5] Polak and Lu[7] Tewari *et al.*[13]	McAuliffe[6] Price[8] Sanemasa *et al.*[9] Sawamura *et al.*[11] Sutton and Calder[12]	
308.2		Sanemasa *et al.*[9]	
318.2		Sanemasa *et al.*[9]	
412.2			Guseva and Parnov[3]
435.2			Guseva and Parnov[3]
480.2			Guseva and Parnov[3]
524.2			Guseva and Parnov[3]

All the experimental and reference data are listed in Table 8 and shown in Fig. 7. The Recommended and Tentative data are shown in Fig. 8.

TABLE 8. Experimental values for solubility of *o*-xylene (1) in water (2)

T/K	Experimental values x_1 (R=recommended, T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
273.2	$2.41 \cdot 10^{-5}$ (D; Ref. 7)	$3.8 \cdot 10^{-5}$
283.2	$3.60 \cdot 10^{-5}$ (T; Ref. 2)	$3.5 \cdot 10^{-5}$
288.2	$2.85 \cdot 10^{-5}$ (T; Ref. 9)	$3.5 \cdot 10^{-5}$
293.2	$4.08 \cdot 10^{-5}$ (T; Ref. 2)	$3.5 \cdot 10^{-5}$
298.1	$3.04 \cdot 10^{-5}$ (T; Ref. 10)	$3.6 \cdot 10^{-5}$
298.2	$3.46 \cdot 10^{-5}$ (R; Ref. 1), $3.78 \cdot 10^{-5}$ (R; Ref. 5), $2.97 \cdot 10^{-5}$ (T; Ref. 6), $3.61 \cdot 10^{-5}$ (R; Ref. 7), $2.83 \cdot 10^{-5}$ (T; Ref. 8), $3.04 \cdot 10^{-5}$ (T; Ref. 9), $4.46 \cdot 10^{-5}$ (T; Ref. 11), $2.89 \cdot 10^{-5}$ (T; Ref. 12), $3.76 \cdot 10^{-5}$ (R; Ref. 13)	$3.6 \cdot 10^{-5}$
308.2	$3.35 \cdot 10^{-5}$ (T; Ref. 9)	$3.8 \cdot 10^{-5}$
318.2	$3.64 \cdot 10^{-5}$ (T; Ref. 9)	$4.1 \cdot 10^{-5}$
412.2	$8.00 \cdot 10^{-5}$ (D; Ref. 3)	$2.5 \cdot 10^{-4}$
435.2	$1.58 \cdot 10^{-4}$ (D; Ref. 3)	$4.5 \cdot 10^{-4}$
480.2	$6.93 \cdot 10^{-4}$ (D; Ref. 3)	$1.4 \cdot 10^{-3}$
524.2	$1.64 \cdot 10^{-3}$ (D; Ref. 3)	$4.3 \cdot 10^{-3}$

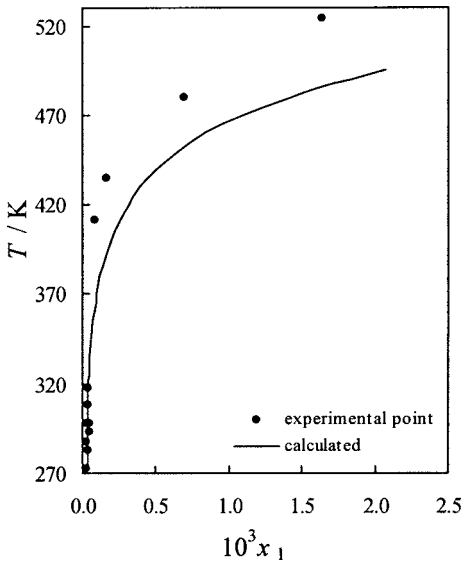

FIG. 7. All the solubility data for *o*-xylene (1) in water (2).

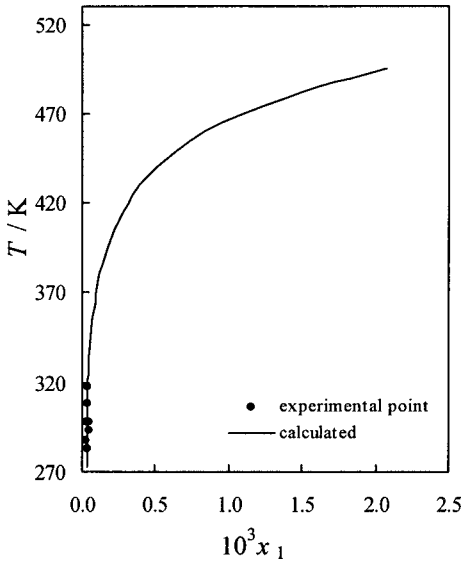

FIG. 8. Recommended and tentative solubility data for *o*-xylene (1) in water (2).

Critical Evaluation of the Solubility of Water (2) in *o*-Xylene (1)

The experimental solubility for (2) in (1) have been investigated by Högfeldt and Bolander[4] at 298 K, and Polak and Lu[7] at 273 and 298 K.

Reference solubility data for (2) in (1) were obtained by the Evaluators using the method described in the Preface to Part 2 and expressed by the equation:

$$\ln x_2 = d_1 + d_2(1/T_r - 1) + d_3(1 - T_r)^{1/3} + d_4(1 - T_r), \quad (2)$$

where $d_1 = -0.332$, $d_2 = -2.775$, $d_3 = -0.027$, $d_4 = -6.308$, and $T_r = T/573.6$.

Equation (2) was used for obtaining the Reference data by regression of the data obtained from those calculated from Reference data of solubility of *o*-xylene in water by the Equation of State with an association term. Comparison between Reference and experimental data is one of the criteria used to assign data to categories.

The experimental and reference solubility data for (2) in (1) are listed in Table 9. The data of Högfeldt and Bolander,[4] and Polak and Lu[7] at 298 K are in good agreement (within 30% relative standard deviation) with each other and with the reference data and are Recommended. The data of Polak and Lu[7] at 273 K are in good agreement (within 30% relative standard deviation) with the reference and are Tentative.

TABLE 9. Experimental values for solubility of water (2) in *o*-xylene (1)

T/K	Experimental values x_2 (T=tentative)	Reference values $x_2 \pm 30\%$
273.2	$1.09 \cdot 10^{-3}$ (T; Ref. 7)	$1.2 \cdot 10^{-3}$
298.2	$2.60 \cdot 10^{-3}$ (R; Ref. 4), $2.68 \cdot 10^{-3}$ (R; Ref. 7)	$2.6 \cdot 10^{-3}$

High Pressure Solubility of *o*-Xylene (1) in Water (2)

The experimental high pressure solubility for (1) in (2) investigated by Sawamura *et al.*[11] at 298 K and 50 000 kPa–250 000 kPa have not been critically evaluated because the developed method is not applied for such data. An evaluation of these data was presented by Hefter and Young.[71]

Rejected and Inaccessible Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga[15] are independent data. The data reported by Alwani and Schneider,[14] lack sufficient information to justify evaluation. Therefore these data are Rejected.

Components:	Original Measurements:
(1) *o*-Xylene; C_8H_{10}; [95-47-6] (2) Water; H_2O; [7732-18-5]	L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **71**, 3644 (1949).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and Z. Maczynska

Experimental Data

The solubility of *o*-xylene in water at 25 °C was reported to be 0.0204 $g(1)$/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is $3.46 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of (1) and (2) was rotated for 20 h in a constant temperature bath at 25 °C. A sample (5–20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10–50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

Source and Purity of Materials:

(1) Eastman Kodak Co. best grade; fractionally distilled; b.p. range 144.3–144.5 °C.
(2) Not specified.

Estimated Error:

Not specified.

References:

[1]L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **71**, 3644 (1949).
[2]A. Ben-Naim and J. Wilf, J. Chem. Phys. **70**, 771 (1979).
[3]A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **18**, 76 (1963).
[4]E. Högfeldt and B. Bolander, Ark. Kemi **21**, 161 (1964).
[5]D. F. Keeley, M. A. Hoffpauir, and J. R. Meriwether, J. Chem. Eng. Data **36**, 456 (1991).
[6]C. McAuliffe, Nature (London) **200**, 1092 (1963).
[7]J. Polak and B. C. Y. Lu, Can. J. Chem. **51**, 4018 (1973).
[8]L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
[9]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).
[10]I. Sanemasa, Y. Miyazaki, S. Arakawa, M. Kumamaru, and T. Deguchi, Bull. Chem. Soc. Jpn. **60**, 517 (1987).
[11]S. Sawamura, K. Suzuki, and Y. J. Taniguchi, J. Solution Chem. **16**, 649 (1987).
[12]C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).
[13]Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).
[14]Z. Alwani and G. M. Schneider, Ber. Bunsen-Ges. Phys. Chem. **73**, 294 (1969).
[15]T. Krzyzanowska and J. Szeliga, Nafta (Katowice) **12**, 413 (1978).

Components:
(1) *o*-Xylene; C_8H_{10} ; [95-47-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. Ben-Naim and J. Wilf, J. Phys. Chem. **70**, 771 (1979).

Variables:
Temperature: 10.0 °C and 20.0 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of *o*-xylene in water

t/°C	$10^3 \cdot$ mol(1)/L sln	$10^2 \cdot g(1)$/100 g sln (compilers)	$10^5 \cdot x_1$ (compilers)
10.0	2.00	2.12	3.60
20.0	2.26	2.40	4.06

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. A saturated solution was diluted several times and the optical density was measured by a Perkin-Elmer Model 450 spectrophotometer in the UV region of 200–400 nm.

Source and Purity of Materials:
(1) Fluka, puriss grade, purity ⩾99.5%; used as received.
(2) Triply distilled.

Estimated Error:
Temperature: ±0.2 °C.
Solubility: 1% (reproducibility of measurements).

Components:
(1) *o*-Xylene; C_8H_{10} ; [95-47-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. N. Guseva and E. I. Parnov, Zh. Fiz. Khim. **37**, 2763 (1963).

Variables:
Temperature: 139 °C–251 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

Solubility of *o*-xylene in water

t/°C	$10^4 \cdot x_1$ (compiler)	$g(1)$/100 g sln
139	0.80	0.047
162	1.58	0.093
207	6.93	0.407
251	16.42	0.960

Auxiliary Information

Method/Apparatus/Procedure:
The measurements were made in sealed glass tubes. No details were reported in the paper.

Source and Purity of Materials:
(1) Source not specified; n_D^{20}=1.5054
(2) Doubly distilled.

Estimated Error:
Not specified.

Components:
(1) *o*-Xylene; C_8H_{10} ; [95-47-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
E. Högfeldt and B. Bolander, Ark. Kemi **21**, 161 (1964).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

The solubility of water in *o*-xylene was reported to be 0.022 mol (2)/L sln.

The corresponding mass percent and mol fraction, x_2 , calculated by the compilers are 0.045 $g(2)$/100 g sln and 0.0026. The assumption that 1.00 L sln=876 g sln was used in the calculation.

Auxiliary Information

Method/Apparatus/Procedure:
The water determination was carried out according to Johansson's modification of the Karl Fischer titration in Hardy *et al.*[1] and Johansson.[2]

Source and Purity of Materials:
(1) Fluka; 0.7% of (*m*-*p*) xylene, 0.07% of ethylbenzene; purity 99.0%; used as received.

Estimated Error:
Temperature: ±0.3 °C.
Solubility: ±0.002mol(2)/L sln (type of error not specified).

References:
[1]C. J. Hardy, B. F. Greenfield, and D. Scargill, J. Chem Soc. 90 (1961).
[2]A. Johansson, Sv. Papperstidn. **11B**, 124 (1947).

Components:
(1) *o*-Xylene; C_8H_{10} ; [95-47-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
D. F. Keeley, M. A. Hoffpauir, and J. R. Meriwether, J. Chem. Eng. Data **36**, 456 (1991).

Variables:
One temperature: 298.15 K

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of *o*-xylene in water

T/K	mol (1)/L sln	$g(1)$/100 g sln (compilers)	x_1 (compilers)
298.15	$(2.09\pm0.05)\cdot10^{-3}$	$2.23\cdot10^{-2}$	$3.78\cdot10^{-5}$

Auxiliary Information

Method/Apparatus/Procedure:
The solubility were determined by a headspace chromatographic analysis, Keeley and Meriwether,[1] using a multiple injection interrupted flow technique. Samples were prepared in septum bottles of 160 mL volume which were thermostatted and shaken for 72 h prior to analysis. For analysis each bottle was transferred to a tempering beaker and pressurized to 15.00 psig with chromatographic grade nitrogen. Bottles were attached to the headspace sampling port of a chromatograph with 1 m by 3.2 mm stainless steel column (5% SP-1200, 1.75% Bentone-34) on 100/1200 mesh Supelcoport (Supelco Inc.) and FID detector. Solubility was calculated on the basis of Henry's law.

Source and Purity of Materials:
(1) Aldrich Gold Label; purity 99.8%; checked by glc; used as received.
(2) Deionized water.

Estimated Error:
Temperature: ±0.05 K.

References:
[1]D. F. Keeley and J. R. Meriwether, Rev. Sci. Instrum. **57**, 1434 (1986).

Components:
(1) *o*-Xylene; C_8H_{10} ; [95-47-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. McAuliffe, Nature (London) **200**, 1092 (1963).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

The solubility of *o*-xylene in water at 25 °C was reported to be 0.0175 $g(1)$/100 g sln.

The corresponding mole fraction, x_1 , calculated by the compilers is $2.97 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:
The saturated solution of (1) in (2) was prepared by either shaking vigorously on a reciprocal shaker or stirring for several days with a magnetic stirrer. A 0.05 mL or 0.10 mL sample of the hydrocarbon-saturated water was injected directly into a gas liquid chromatograph.

Source and Purity of Materials:
(1) Phillips Petroleum Co.; 99+%; used as received.
(2) Distilled.

Estimated Error:
Temperature: ±1.5 °C.
Solubility: 0.0008 (standard deviation of mean).

Components:
o-Xylene; C_8H_{10} ; [95-47-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. Polak and B. C.-Y. Lu, Can. J. Chem. **51**, 4018 (1973).

Variables:
Temperature: 0 °C–25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

Solubility of *o*-xylene in water

t/°C	$10^5 \cdot x_1$ (compiler)	$g(1)$/100 g sln (compiler)	mg (1)/kg (2)
0[a]	2.41	0.0142	142[c]
25[b]	3.61	0.0213	213[c]

Solubility of water in *o*-xylene

t/°C	$10^3 \cdot x_2$ (compiler)	$g(2)$/100 g (compiler)	mg (2)/kg (1)
0[a]	1.09	0.0185	185[d]
25[b]	2.68	0.0456	456[e]

[a–e]See Estimated Error.

Auxiliary Information

Method/Apparatus/Procedure:
Approximately 50 mL of (1) together with (2) were placed in a 125 mL Hypo-vial which was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 h and left in the bath for 3 days or was kept in the bath without stirring for 7 days, before samples were taken for analysis.

The solubility of water in the organic layer was determined by the Karl Fischer titration and the solubility of hydrocarbon in the water layer was determined by gas chromatography.

Source and Purity of Materials:
Eastman Organics, pure grade reagent; shaken three times with distilled water.
(2) Distilled.

Estimated Error:
Temperature: (a) ±0.02 °C, (b) ±0.01 °C.
Solubility: (c) ±1.7%, (d) ±4.7%, (e) ±3.1% (from two or three determinations).

Components:
(1) *o*-Xylene; C_8H_{10} ; [95-47-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).

Variables:
Temperature: 15 °C–45 °C

Prepared By:
G. T. Hefter

Experimental Data

Solubility of *o*-xylene in water

t/°C	$10^5 \cdot x_1$ (compiler)[a]	$g(1)$/100 g sln (compiler)[a]	$10^3 \cdot$ mol(1)/L sln
15	2.85	0.0168	1.58 ± 0.11
25	3.04	0.0179	1.68 ± 0.06
35	3.35	0.0198	1.85 ± 0.02
45	3.64	0.0214	2.00 ± 0.02

[a]Assuming solution densities to be the same as those of pure water at the same temperature (Kell[1]).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to an earlier design (Sanemasa *et al.*[2]) and is described in detail in the paper. 100–200 mL of (2) and 10–20 mL of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was established a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 mL aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.

Source and Purity of Materials:
(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 98.0%, used without further purification.
(2) Redistilled; no further details given.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: see table, type of error not specified.

References:
[1]G. S. Kell, J. Chem. Eng. Data **20**, 97 (1975).
[2]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Chem. Lett. 225 (1981).

Components:
(1) *o*-Xylene; C_8H_{10} ; [95-47-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

The solubility of *o*-xylene in water at 25 °C and at system pressure was reported to be 167.0 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are $0.0167g(1)$/100 g sln and $2.83 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and ensured saturation of the (2) phase in 2–4 days. Analyses were carried out by glc using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

Source and Purity of Materials:
(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.
(2) Distilled.

Estimated Error:
Temperature: ±1 °C.
Solubility: ±4.0 mg(1)/kg(2).

Components:
(1) *o*-Xylene; C_8H_{10} ; [95-47-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. Sanemasa, Y. Miyazaki, S. Arakawa, M. Kumamaru, and T. Deguchi, Bull. Chem. Soc. Jpn. **60**, 517 (1987).

Variables:
One temperature: 25.0 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of *o*-xylene in water

t/°C	mol (1)/L sln	g(1)/100 g sln (compilers)	x_1 (compilers)
25.0	$1.68 \cdot 10^{-3}$	$1.79 \cdot 10^{-2}$	$3.04 \cdot 10^{-5}$

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. The apparatus used for preparing aqueous solutions saturated with hydrocarbon vapor was the same as that previously reported in Sanemasa *et al.*[1] The method was based on the introduction of phase (1) (by bubbling air through the mixture using circulating pump in a closed system) into 100 mL of water. After 10 min (at circulation rate of vapor of 1.5 L/min) equilibrium was attained, and a 30 mL portion of the saturated aqueous solution was transferred into three separatory funnels with 5 mL of toluene. Mixtures were analyzed by gas chromatography.

Source and Purity of Materials:
(1) Source not specified; analytical reagent grade; purity 98%; used as received.
(2) Deionized and redistilled.

Estimated Error:
Temperature: ±0.1 °C.

References:
[1]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).

Components:
(1) *o*-Xylene; C_8H_{10} ; [95-47-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
S. Sawamura, K. Suzuki, and Y. Taniguchi, J. Solution Chem. **16**, 649 (1987).

Variables:
One temperature: 25.00 °C
Pressure: 0.1 MPa–250 MPa

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of *o*-xylene in water

t/°C	P/MPa	x_p/x_0	g(1)/100 g sln (compilers)	$10^5 \cdot x_1$ (compilers)
25.00	0.1	1	0.02616	4.44
	50	1.077	0.02816	4.78
	100	1.132	0.02964	5.03
	150	1.125	0.02940	4.99
	200	1.102	0.02881	4.89
	250	1.056	0.02763	4.69

x_p/x_0=relation of solubilities at high and normal pressure.

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. Water (2) and a few drops of hydrocarbon (1) were placed in a high pressure optical cell with a Teflon ball for stirring. The sample was pressurized and shaken in a thermoregutated water bath for 5–20 h. Details of the apparatus, procedures, and purification were reported in Sawamura *et al.*[1] Solubilities were calculated by the compilers on the basis of absorbance measurements and the solubility value at 25 °C and 0.1 MPa.

Source and Purity of Materials:
(1) Nakarai Chem. (Japan); shaken successively with H_2SO_4, NaOH, H_2O, dried over $CaCl_2$, distilled.
(2) Deionized; distilled with a trace of $KMnO_4$.

Estimated Error:
Temperature: ±0.05 °C.

References:
[1]S. Sawamura, M. Tsuchiya, Y. Taniguchi, and K. Suzuki, Physica **139**, 732 (1986).

Components:
(1) *o*-Xylene; C_8H_{10} ; [95-47-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

The solubility of *o*-xylene in water at 25 °C was reported to be 170.5 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.01705 $g(1)/100$ g sln and $2.892 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:
The concentration of (1) in (2) was determined by gas chromatography.

Source and Purity of Materials:
(1) Aldrich Chemical Co. or Matheson, Coleman, and Bell 99+%.
(2) Distilled.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: 2.5 mg (1)/kg (2) (standard deviation of the mean for six replicates).

Components:
(1) *o*-Xylene; C_8H_{10} ; [95-47-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

Variables:
One temperature: 25.0 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of *o*-xylene in water

t/°C	mol (1)/L sln	$g(1)/100$ g sln (compilers)	x_1 (compilers)
25.0	$2.08 \cdot 10^{-3}$	$2.22 \cdot 10^{-2}$	$3.76 \cdot 10^{-5}$

Auxiliary Information

Method/Apparatus/Procedure:
A generator column method was used, as described in DeVoe *et al.*[1] and May *et al.*[2] A column was coated with (1) by pulling about 2 mL of liquid through the clean dry support (Chromosorb W-HP). A saturated solution was generated by pumping water into the inlet of the coated column and was then analyzed by hplc. The column was thermostated by pumping water from a bath through a column jacket. An average of at least three measurements is reported.

Source and Purity of Materials:
(1) Source not specified; purity >99 mole % checked by high-temperature glc.
(2) Source not specified.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: 1% (estimated by the authors).

References:
[1]H. De Voe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. (USA) **86**, 361 (1981).
[2]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).

2.4. *m*-Xylene+Water

Components:
(1) *m*-Xylene (1,3-dimethylbenzene); C_8H_{10} ; [108-38-3]
(2) Water; H_2O; [7732-18-5]

Evaluators:
A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, January, 2004.

Critical Evaluation of the Solubility of *m*-Xylene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below together with temperature range and pressure range, if reported:

Author (s)	*T*/K	Author (s)	*T*/K
Anderson and Prausnitz[1]	374–473 (101–2004 kPa)	Price[11]	298
Andrews and Keefer[2]	298	Pryor and Jentoft[12]	341–544
Bohon and F. Claussen[3]	298	Sanemasa *et al.*[13]	288–318
	293–343	Sanemasa *et al.*[14]	298
Guseva and Parnov[6]	400–512	Sawamura *et al.*[15]	298
Keeley *et al.*[8]	298	Sutton and Calder[16]	298
Miller and Hawthorne[9]	298–473 (6000 kPa)	Tewari *et al.*[17]	298
Polak and Lu[10]	273 and 298	Vesala[18]	298

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 2 and expressed by the equation:

$$\ln x_1 = \ln x_{\min,1} + D[(T_{\min}/T)\ln(T_{\min}/T) + 1 - (T_{\min}/T)], \quad (1)$$

where $\ln x_{\min,1} = -10.52$, $D = 41.5$, and $T_{\min} = 290$.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the Reference data. Comparison between Reference and experimental data is one of the criteria used to assign data to the categories listed in Table 10.

TABLE 10. The data categories for solubility of *m*-xylene (1) in water (2)

T/K	Recommended [data in good agreement (±30%) with each other and with the reference data]	Tentative [data in good agreement (±30%) with the reference data]	Doubtful [data in poor agreement (>30%) with the reference data]
273.2		Polak and Lu[10]	
288.2		Sanemasa *et al.*[13]	
293.2		Chernoglazova and Simulin[4]	
298.0		Miller and Hawthorne[9] Vesala[18]	
298.1		Sanemasa *et al.*[14]	
298.2	Andrews and Keefer[2] Keeley *et al.*[8] Polak and Lu[10] Sanemasa *et al.*[13] Sawamura *et al.*[15] Tewari *et al.*[17]	Bohon and F. Claussen[3] Price[11] Sutton and Calder[16]	
308.2		Sanemasa *et al.*[13]	
313.2		Chernoglazova and Simulin[4]	
318.2		Sanemasa *et al.*[13]	
323.0		Miller and Hawthorne[9]	
340.9			Pryor and Jentoft[12]
343.2			Chernoglazova and Simulin[4]
373.0		Miller and Hawthorne[9]	
373.6			Anderson and Prausnitz[1]
378.8		Pryor and Jentoft[12]	
397.4		Pryor and Jentoft[12]	
398.2			Anderson and Prausnitz[1]
398.3			Anderson and Prausnitz[1]
400.2			Guseva and Parnov[6]
422.2			Guseva and Parnov[6]
423.0		Miller and Hawthorne[9]	
423.2		Anderson and Prausnitz[1]	
437.4		Pryor and Jentoft[12]	
448.4		Anderson and Prausnitz[1]	
459.6		Pryor and Jentoft[12]	
460.2			Guseva and Parnov[6]
463.1		Pryor and Jentoft[12]	
473.0		Miller and Hawthorne[9]	
473.4		Anderson and Prausnitz[1]	
512.2			Guseva and Parnov[6]
539.8		Pryor and Jentoft[12]	
543.8		Pryor and Jentoft[12]	

All the experimental and reference data are listed in Table 11 and shown in Fig. 9. The Recommended and Tentative data are shown in Fig. 10.

TABLE 11. Experimental values for solubility of *m*-xylene (1) in water (2)

T/K	P/kPa	Experimental values x_1 (R=recommended, T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
273.2		$3.32 \cdot 10^{-5}$ (T; Ref. 10)	$2.9 \cdot 10^{-5}$
288.2		$2.68 \cdot 10^{-5}$ (T; Ref. 13)	$2.7 \cdot 10^{-5}$
293.2		$2.70 \cdot 10^{-5}$ (T; Ref. 4)	$2.7 \cdot 10^{-5}$
298.0	6000 (Ref. 9)	$2.90 \cdot 10^{-5}$ (T; Ref. 9), $3.49 \cdot 10^{-5}$ (T; Ref. 18)	$2.7 \cdot 10^{-5}$
298.1		$2.40 \cdot 10^{-5}$ (T; Ref. 14)	$2.7 \cdot 10^{-5}$
298.2	100 (Ref. 15)	$2.93 \cdot 10^{-5}$ (R; Ref. 2), $3.33 \cdot 10^{-5}$ (T; Ref. 3), $2.86 \cdot 10^{-5}$ (R; Ref. 8), $2.75 \cdot 10^{-5}$ (R; Ref. 10), $2.27 \cdot 10^{-5}$ (T; Ref. 11), $2.75 \cdot 10^{-5}$ (R; Ref. 13), $2.70 \cdot 10^{-5}$ (R; Ref. 15), $2.48 \cdot 10^{-5}$ (T; Ref. 16), $2.73 \cdot 10^{-5}$ (R; Ref. 17)	$2.7 \cdot 10^{-5}$
308.2		$2.85 \cdot 10^{-5}$ (T; Ref. 13)	$2.9 \cdot 10^{-5}$
313.2		$3.70 \cdot 10^{-5}$ (T; Ref. 4)	$3.0 \cdot 10^{-5}$
318.2		$3.15 \cdot 10^{-5}$ (T; Ref. 13)	$3.2 \cdot 10^{-5}$
323.0	6000 (Ref. 9)	$3.60 \cdot 10^{-5}$ (T; Ref. 9)	$3.4 \cdot 10^{-5}$
340.9		$5.90 \cdot 10^{-5}$ (D; Ref. 12)	$4.4 \cdot 10^{-5}$
343.2		$6.40 \cdot 10^{-5}$ (D; Ref. 4)	$4.6 \cdot 10^{-5}$
373.0	6000 (Ref. 9)	$8.50 \cdot 10^{-5}$ (T; Ref. 9)	$8.2 \cdot 10^{-5}$
373.6	101 (Ref. 1)	$1.38 \cdot 10^{-4}$ (D; Ref. 1)	$8.3 \cdot 10^{-5}$
378.8		$1.127 \cdot 10^{-4}$ (T; Ref. 12)	$9.3 \cdot 10^{-5}$
397.4		$1.749 \cdot 10^{-4}$ (T; Ref. 12)	$1.4 \cdot 10^{-4}$
398.2	281 (Ref. 1)	$2.04 \cdot 10^{-4}$ (D; Ref. 1)	$1.5 \cdot 10^{-4}$
398.3	274 (Ref. 1)	$2.00 \cdot 10^{-4}$ (D; Ref. 1)	$1.5 \cdot 10^{-4}$
400.2		$5.30 \cdot 10^{-5}$ (D; Ref. 6)	$1.5 \cdot 10^{-4}$
422.2		$1.22 \cdot 10^{-4}$ (D; Ref. 6)	$2.7 \cdot 10^{-4}$
423.0	6000 (Ref. 9)	$2.70 \cdot 10^{-4}$ (T; Ref. 9)	$2.7 \cdot 10^{-4}$
423.2	598 (Ref. 1)	$2.98 \cdot 10^{-4}$ (T; Ref. 1)	$2.7 \cdot 10^{-4}$
437.4		$4.265 \cdot 10^{-4}$ (T; Ref. 12)	$3.9 \cdot 10^{-4}$
448.4	1142 (Ref. 1)	$5.17 \cdot 10^{-4}$ (T; Ref. 1)	$5.2 \cdot 10^{-4}$
459.6		$7.825 \cdot 10^{-4}$ (T; Ref. 12)	$7.0 \cdot 10^{-4}$
460.2		$2.85 \cdot 10^{-4}$ (D; Ref. 6)	$7.1 \cdot 10^{-4}$
463.1		$7.762 \cdot 10^{-4}$ (T; Ref. 12)	$7.7 \cdot 10^{-4}$
473.0	6000 (Ref. 9)	$8.80 \cdot 10^{-4}$ (T; Ref. 9)	$1.0 \cdot 10^{-3}$
473.4	2004 (Ref. 1)	$9.64 \cdot 10^{-4}$ (T; Ref. 1)	$1.0 \cdot 10^{-3}$
512.2		$1.11 \cdot 10^{-3}$ (D; Ref. 6)	$2.8 \cdot 10^{-3}$
539.8		$4.956 \cdot 10^{-3}$ (T; Ref. 12)	$5.7 \cdot 10^{-3}$
543.8		$5.00 \cdot 10^{-3}$ (T; Ref. 12)	$6.3 \cdot 10^{-3}$

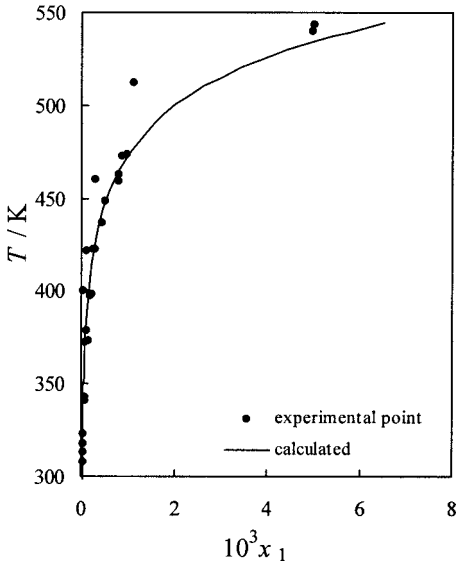

FIG. 9. All the solubility data for *m*-xylene (1) in water (2).

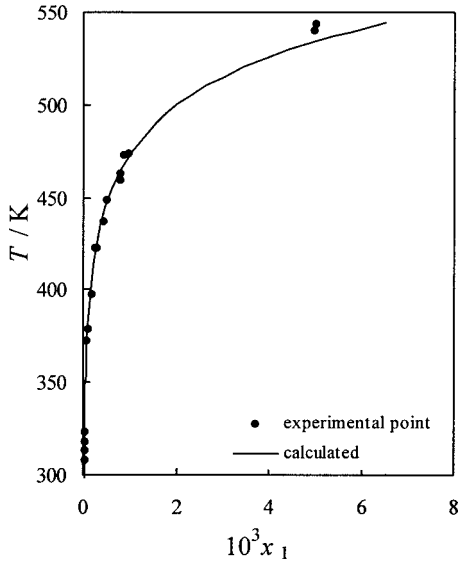

FIG. 10. Recommended and tentative solubility data for *m*-xylene (1) in water (2).

Critical Evaluation of the Solubility of Water (2) in *m*-Xylene (1)

The experimental solubility data for (2) in (1) have been investigated by the authors listed below together with temperature range and pressure range, if reported:

Author (s)	*T*/K	Author (s)	*T*/K
Anderson and Prausnitz[1]	374–473 (101–2004 kPa)	Högfeldt and Bolander[7]	298
Chernoglazova and Simulin[4]	293–343	Polak and Lu[10]	273–298
Englin *et al.*[5]	283–303		

Reference solubility data for (2) in (1) were obtained by the Evaluators using the method described in the Preface to Part 2 and expressed by the equation:

$$\ln x_2 = d_1 + d_2(1/T_r - 1) + d_3(1 - T_r)^{1/3} + d_4(1 - T_r), \quad (2)$$

where $d_1 = -0.383$, $d_2 = -3.168$, $d_3 = -0.019$, $d_4 = -5.636$, and $T_r = T/566.8$.

Equation (2) was used for obtaining the Reference data by regression of the data obtained from those calculated from Reference data of solubility of *m*-xylene in water by the Equation of State with an association term. Comparison between Reference and experimental data is one of the criteria used to assign data to the categories listed in Table 12.

TABLE 12. The data categories for solubility of water (2) in *m*-xylene (1)

T/K	Recommended [data in good agreement (±30%) with each other and with the reference data]	Tentative [data in good agreement (±30%) with the reference data]
273.2		Polak and Lu[10]
283.2		Englin *et al.*[5]
293.2	Chernoglazova and Simulin[4] Englin *et al.*[5]	
298.2	Högfeldt and Bolander[7] Polak and Lu[10]	
303.2		Englin *et al.*[5]
313.2		Chernoglazova and Simulin[4]
343.2		Chernoglazova and Simulin[4]
373.6		Anderson and Prausnitz[1]
398.2		Anderson and Prausnitz[1]
398.3		Anderson and Prausnitz[1]
423.2		Anderson and Prausnitz[1]
448.4		Anderson and Prausnitz[1]
473.4		Anderson and Prausnitz[1]

The experimental and reference solubility data for (2) in (1) are listed in Table 13 and shown in Fig. 11.

TABLE 13. Experimental values for solubility of water (2) in *m*-xylene (1)

T/K	Experimental values x_2 (R=recommended, T=tentative)	Reference values $x_2 \pm 30\%$
273.2	$1.11 \cdot 10^{-3}$ (T; Ref. 10)	$1.2 \cdot 10^{-3}$
283.2	$1.70 \cdot 10^{-3}$ (T; Ref. 5)	$1.7 \cdot 10^{-3}$
293.2	$2.00 \cdot 10^{-3}$ (R; Ref. 4), $2.37 \cdot 10^{-3}$ (R; Ref. 5)	$2.3 \cdot 10^{-3}$
298.2	$2.60 \cdot 10^{-3}$ (R; Ref. 7), $2.54 \cdot 10^{-3}$ (R; Ref. 10)	$2.7 \cdot 10^{-3}$
303.2	$3.15 \cdot 10^{-3}$ (T; Ref. 5)	$3.1 \cdot 10^{-3}$
313.2	$3.90 \cdot 10^{-3}$ (T; Ref. 4)	$4.1 \cdot 10^{-3}$
343.2	$1.11 \cdot 10^{-2}$ (T; Ref. 4)	$9.2 \cdot 10^{-3}$
373.6	$1.647 \cdot 10^{-2}$ (T; Ref. 1)	$1.9 \cdot 10^{-2}$
398.2	$2.785 \cdot 10^{-2}$ (T; Ref. 1)	$3.3 \cdot 10^{-2}$
398.3	$2.857 \cdot 10^{-2}$ (T; Ref. 1)	$3.3 \cdot 10^{-2}$
423.2	$5.131 \cdot 10^{-2}$ (T; Ref. 1)	$5.5 \cdot 10^{-2}$
448.4	$8.840 \cdot 10^{-2}$ (T; Ref. 1)	$9.0 \cdot 10^{-2}$
473.4	$1.510 \cdot 10^{-1}$ (T; Ref. 1)	$1.4 \cdot 10^{-1}$

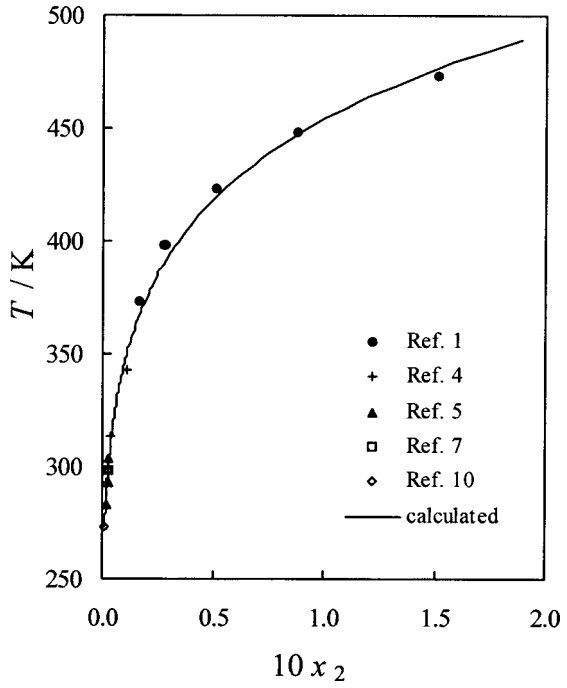

FIG. 11. All the solubility data for water (2) in *m*-xylene (1).

High Pressure Solubility of *m*-Xylene (1) in Water (2)

The experimental high pressure solubility for (1) in (2) investigated by Sawamura *et al.*[15] at 298 K and 50 000 kPa–385 000 kPa have not been critically evaluated because the developed method is not applied for such data. An evaluation of these data was presented by Hefter and Young.[71]

Rejected and Inaccessible Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga[20] are independent data. The data reported by Gill *et al.*[19] lack sufficient information to justify evaluation. Therefore these data are Rejected.

Components: (1) *m*-Xylene; C_8H_{10} ; [108-38-3] (2) Water; H_2O; [7732-18-5]	**Original Measurements:** F. E. Anderson and J. M. Prausnitz, Fluid Phase Equilib. **32**, 63 (1986).
Variables: Temperature: 99.4 °C–200.4 °C Pressure: 1.53 bar–23.63 bar	**Prepared By:** A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of *m*-xylene in water

t/°C	*P*/bar	*g*(1)/100 g sln (compilers)	$10^3 \cdot x_1$
100.4	1.01	0.081	1.38 ± 0.15
125.0	2.81	0.120	2.04 ± 0.14
125.1	2.74	0.118	2.00 ± 0.16
150.0	5.98	0.175	2.98 ± 0.15
175.2	11.42	0.304	5.17 ± 0.17
200.2	20.04	0.565	9.64 ± 0.62

Solubility of water in *m*-xyle

t/°C	*P*/bar	*g*(2)/100 g sln (compilers)	x_2
100.4	1.01	0.283	0.01647 ± 0.00051
125.0	2.81	0.484	0.02785 ± 0.00027
125.1	2.74	0.497	0.02857 ± 0.00077
150.0	5.98	0.909	0.05131 ± 0.00052
175.2	11.42	1.619	0.08840 ± 0.00065
200.2	20.04	2.930	0.1510 ± 0.00092

Auxiliary Information

Method/Apparatus/Procedure:

The analytical method was used. The equilibrium cell, about 140 mL, was filled with a mixture of (1) and (2), temperature controllers were set at the desired temperature, liquids were degassed, agitated and allowed to reach equilibrium for 2 h. Details of the apparatus and sampling procedures were described in the paper. Temperatures were measured by a resistance temperature detector. All analysis were made using a gas chromatograph equipped with a thermal-conductivity detector. Mean values of 5–9 replicated measurements were reported.

Source and Purity of Materials:

(1) Source not specified; spectral grade reagent; used as received.
(2) Purified and deionized by adsorption on activated carbon.

Estimated Error:

Temperature: ± 0.5 °C.
Solubility: standard deviation as above.
Pressure: ± 0.1 bar.

References:

[1]F. E. Anderson and J. M. Prausnitz, Fluid Phase Equilib. **32**, 63 (1986).
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[14]I. Sanemasa, Y. Miyazaki, S. Arakawa, M. Kumamaru, and T. Deguchi, Bull. Chem. Soc. Jpn. **60**, 517 (1987).
[15]S. Sawamura, K. Suzuki, and Y. J. Taniguchi, J. Solution Chem. **16**, 649 (1987).
[16]C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).
[17]Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).
[18]A. Vesala, Acta Chem. Scand., Ser. A **28**, 839 (1974).
[19]S. J. Gill, N. F. Nichols, and I. Wadso, J. Chem. Thermodyn. **8**, 445 (1976).
[20]T. Krzyzanowska and J. Szeliga, Nafta (Katowice) **12**, 413 (1978).

Components:
(1) *m*-Xylene; C_8H_{10} ; [108-38-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **71**, 3644 (1949).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

The solubility of *m*-xylene in water at 25 °C was reported to be 0.010173 $g(1)$/100 g sln.

The corresponding mole fraction, x_1 , calculated by the compilers is $2.93 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:
A mixture of (1) and (2) was rotated for 20 h in a constant temperature bath at 25 °C. A sample (5–20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10–50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

Source and Purity of Materials:
(1) Eastman Kodak Co. best grade; fractionally distilled; b.p. 139.5 °C.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) *m*-Xylene; C_8H_{10} ; [108-38-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. L. Bohon and W. F. Claussen, J. Am. Chem. Soc. **73**, 1571 (1951).

Variables:
Temperature: 0.4 °C–39.6 °C

Prepared By:
G. T. Hefter

Experimental Data

Solubility of *m*-xylene in water

t/°C	$10^5 \cdot x_1$ (compiler)	$g(1)$/100 g sln[a] (compiler)
0.4	3.54	0.0209
5.2	3.41	0.0201
14.9	3.25	0.0192
21.0	3.33	0.0196
25.0	3.33[b]	0.0196[b]
25.6	3.33	0.0196
30.3	3.36	0.0198
34.9	3.44	0.0203
39.6	3.69	0.0218

[a]Solubilities of (1) in (2) were reported as ''optical density'' (absorbance) measurements. Solubilities were calculated by the compiler using the Beer-Lambert law, the stated cell path length (1 cm) and the authors' ''extinction coefficients'' (absorptivities) and corrected optical densities. This gave a solubility of $g(1)$/L sln which was then converted to $g(1)$/100 g sln by assuming a solution density of 1.00 kg/L.

[b]Given in the original paper as 0.196 $g(1)$/L sln.

Auxiliary Information

Method/Apparatus/Procedure:
A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24 h and then allowed to settle for at least another 24 h. Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been tarred, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of the samples were inserted into a quartz cuvette and measured in a Beckman DU spectrophotometer. Absorbances were corrected for adsorption of (1) onto the walls of the cuvette.

Source and Purity of Materials:
(1) Oronite Chemical Co. was sulfonated, hydrolyzed, steam distilled, washed, dried by passing through silica gel and finally distilled. Purity was judged by refractometry (no value given).
(2) Air-free conductivity water (no details given).

Estimated Error:
Temperature: ±0.02 °C.
Solubility: ±0.5% relative.

Components:
(1) *m*-Xylene; C_8H_{10} ; [108-38-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
F. S. Chernoglazova and Yu. N. Simulin, Zh. Fiz. Khim. **50**, 809 (1976).

Variables:
Temperature: 20 °C–70 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

Solubility of *m*-xylene in water

t/°C	$10^5 \cdot x_1$ (compiler)	$g(1)$/100 g sln
20	2.7	0.016
40	3.7	0.022
70	6.4	0.038

Solubility of water in *m*-xylene

t/°C	$10^3 \cdot x_2$ (compiler)	$g(2)$/100 g sln
20	2.0	0.034
40	3.9	0.067
70	11.1	0.190

Auxiliary Information

Method/Apparatus/Procedure:
The solubility of (1) in (2) was determined by the synthetic method of Fühner.[1] Glass tubes filled with 50–100 mL of (2) were frozen and then (1) was micropipetted. Next, the tubes were sealed and thermostatted for 6 h at 70 °C and 72 h at 20 °C. The solubility was followed visually. The samples were incremented at regular steps 0.005 $g(1)$/100 g(2). The mean value from 5–6 determinations was adopted.

The solubility of (2) in (1) was determined by gas chromatography. A LKhM-7 instrument equipped with a katharometer was employed.

Source and Purity of Materials:
(1) Source not specified; 99.9% purity by glc.
(2) Distilled.

Estimated Error:
Not specified.

References:
[1]H. Fühner, Chem. Ber. **57**, 514 (1924).

Components:
(1) *m*-Xylene; C_8H_{10} ; [108-38-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
B. A. Englin, A. F. Plate, V. M. Tugolukov, and M. A. Pryanishnikova, Khim. Tekhnol. Topl. Masel **10**, 42 (1965).

Variables:
Temperature: 10 °C–30 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

Solubility of *m*-xylene in water

t/°C	$10^3 \cdot x_2$ (compiler)	$g(2)$/100 g sln (compiler)
10	1.70	0.0289
20	2.37	0.0402
30	3.15	0.0536

Auxiliary Information

Method/Apparatus/Procedure:
Component (1) was introduced into a thermostatted flask and saturated for 5 h with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

Source and Purity of Materials:
(1) Not specified.
(2) Not specified.

Estimated Error:
Not specified.

Components:	**Original Measurements:**
(1) *m*-Xylene; C_8H_{10} ; [108-38-3] (2) Water; H_2O; [7732-18-5]	A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **18**, 76 (1963).
Variables:	**Prepared By:**
Temperature: 127 °C–239 °C	A. Maczynski and Z. Maczynska

Experimental Data

Solubility of *m*-xylene in water

t/°C	$10^4 \cdot x_1$ (compiler)	$g(1)$/100 g sln
127	0.53	0.031
149	1.22	0.072
187	2.85	0.168
239	11.06	0.648

Auxiliary Information

Method/Apparatus/Procedure:

The measurements were made in sealed glass tubes. No details were reported in the paper.

Source and Purity of Materials:

(1) Source not specified; n_D^{20}=1.4974.
(2) Doubly distilled.

Estimated Error:

Not specified.

Components:	**Original Measurements:**
(1) *m*-Xylene; C_8H_{10} ; [108-38-3] (2) Water; H_2O; [7732-18-5]	E. Högfeldt and B. Bolander, Ark. Kemi **21**, 161 (1964).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and Z. Maczynska

Experimental Data

The solubility of water in *m*-xylene was reported to be 0.021 mol (2)/L sln.

The corresponding mass percent and mol fraction, x_2, calculated by the compilers are 0.044 $g(2)$/100 g sln and 0.0026. The assumption that 1.00 L sln=860 g sln was used in the calculation.

Auxiliary Information

Method/Apparatus/Procedure:

The water determination was carried out according to Johansson's modification of the Karl Fischer titration in Hardy *et al.*[1] and Johansson.[2]

Source and Purity of Materials:

(1) Fluka; 0.3% of ethylbenzene, 0.03% of *o*-xylene; purity 99.6%; used as received.
(2) Not specified.

Estimated Error:

Temperature: ±0.03 °C.
Solubility: ±0.001 mol(2)/L sln (type of error not specified).

References:

[1]C. J. Hardy, B. F. Greenfield, and D. Scargill, J. Chem Soc. 90 (1961).
[2]A. Johansson, Sv. Papperstidn. **11B**, 124 (1947).

Components:
(1) *m*-Xylene; C_8H_{10} ; [108-38-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
D. F. Keeley, M. A. Hoffpauir, and J. R. Meriwether, J. Chem. Eng. Data **36**, 456 (1991).

Variables:
One temperature: 298.15 K

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of *m*-xylene in water

T/K	mol (1)/L sln	g(1)/100 g sln (compilers)	x_1 (compilers)
298.15	$(1.58 \pm 0.02) \cdot 10^{-3}$	$1.68 \cdot 10^{-2}$	$2.86 \cdot 10^{-5}$

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was determined by a headspace chromatographic analysis, Keeley and Meriwether,[1] using a multiple injection interrupted flow technique. Samples were prepared in septum bottles of 160 mL volume which were thermostatted and shaken for 72 h prior to analysis. For analysis each bottle was transferred to a tempering beaker and pressurized to 15.00 psig with chromatographic grade nitrogen. Bottles were attached to the headspace sampling port of a chromatograph with a 1 m by 3.2 mm stainless steel column (5% SP-1200, 1.75% Bentone-34) on 100/1200 mesh Supelcoport (Supelco Inc.) and FID detector. Solubility was calculated on the basis of Henry's law.

Source and Purity of Materials:
(1) Two samples were used: Baker, purity 99.60% checked by glc, used as received; and Aldrich, purity 99.8% checked by glc, used as received.
(2) Deionized water.

Estimated Error:
Temperature: ± 0.05 K.

References:
[1]D. F. Keeley and J. R. Meriwether, Rev. Sci. Instrum. **57**, 1434 (1986).

Components:
(1) *m*-Xylene; C_8H_{10} ; [108-38-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
D. J. Miller and S. B. Hawthorne, J. Chem. Eng. Data **45**, 78 (2000).

Variables:
Temperature: 298.0 K–473.0 K
Pressure: 60 bar

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of *m*-xylene in water

T/K	P/bar	g(1)/100 g sln (compilers)	$10^4 \cdot x_1$
298.0	60	0.0171	0.29 ± 0.01
323.0	60	0.0212	0.36 ± 0.01
373.0	60	0.0501	0.85 ± 0.04
423.0	60	0.159	2.7 ± 0.1
473.0	60	0.516	8.8 ± 0.2

Auxiliary Information

Method/Apparatus/Procedure:
The dynamic method described in Miller and Hawthorne[1] was used. A high-pressure saturation cell was filled with component (1) and placed in the oven of gas chromatograph to provide precise temperature control. Next water was pumped into the saturation cell. After a 60 min equilibration 10 fractions were collected for 3 min each. The details of filling procedure, equilibration and sampling were described in the paper. The analyses were performed using an HP model 5890 gas chromatograph with flame ionization detection.

Source and Purity of Materials:
(1) Sigma-Aldrich, Milwaukee, WI; purity >99%; used as received.
(2) Not stated.

Estimated Error:
Temperature: ± 0.1 K.
Solubility: as above.

References:
[1]D. J. Miller and S. B. Hawthorne, Anal. Chem. **70**, 1618 (1998).

Components:
(1) *m*-Xylene; C_8H_{10} ; [108-38-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. Polak and B. C.-Y. Lu, Can. J. Chem. **51**, 4018 (1973).

Variables:
Temperature: 0 °C–25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

Solubility of *m*-xylene in water

t/°C	$10^5 \cdot x_1$ (compiler)	*g*(1)/100 g sln (compiler)	mg (1)/kg (2)
0[a]	3.32	0.0196	196[c]
25[b]	2.75	0.0162	162[c]

Solubility of water in *m*-xylene

t/°C	$10^3 \cdot x_2$ (compiler)	*g*(2)/100 g sln (compiler)	mg (2)/kg (1)
0[a]	1.11	0.0188	188[d]
25[b]	2.54	0.0432	432[e]

[a–e]See Estimated Error.

Auxiliary Information

Method/Apparatus/Procedure:
Approximately 50 mL of (1) together with (2) were placed in a 125 mL Hypo-vial which was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 h and left in the bath for 3 days or was kept in the bath without stirring for 7 days, before samples were taken for analysis.

The solubility of water in the organic layer was determined by the Karl Fischer titration and the solubility of hydrocarbon in the water layer was determined by gas chromatography.

Source and Purity of Materials:
(1) Phillips Petroleum o.; pure grade reagent 99+%; shaken three times with distilled water.
(2) Distilled.

Estimated Error:
Temperature: (a) ±0.02 °C, (b) ±0.01 °C.
Solubility: (c) ±1.7%, (d) ±4.7%, (e) ±3.1%
(from two or three determinations).

Components:
(1) *m*-Xylene; C_8H_{10} ; [108-38-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

The solubility of *m*-xylene in water at 25 °C and at system pressure was reported to be 134.0 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 0.0134 *g*(1)/100 g sln and $2.27 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2–4 days. Analyses were carried out by glc using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

Source and Purity of Materials:
(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.
(2) Distilled.

Estimated Error:
Temperature: ±1 °C.
Solubility: ±2.0 mg(1)/kg(2).

Components:
(1) *m*-Xylene; C_8H_{10} ; [108-38-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. A. Pryor and R. E. Jentoft, J. Chem. Eng. Data **6**, 36 (1961).

Variables:
Temperature: 67.7 °C–270.6 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

Solubility of *m*-xylene in water

t/°C	$10^3 \cdot x_1$ (compiler)	*g*(1)/100 g sln (compiler)
67.7	0.0590	0.0348
107.3	0.1127	0.0664
124.2	0.1749	0.1031
164.2	0.4265	0.2509
186.4	0.7825	0.4595
189.9	0.7762	0.4559
266.6	4.956	2.852
270.6	5.00	2.88

Auxiliary Information

Method/Apparatus/Procedure:
Mixtures of (1) and (2) were carefully weighed into glass ampoules. The ampoules were sealed allowing just enough space for thermal expansion. An ampoule, observed through a telescope from behind a safety barrier, was suspended in a 4 L stirred silicone oil bath, and the bath was heated until (1) dissolved. On cooling, a cloud of fine (1) droplets appeared, making the suspension opaque. The temperature was raised until the cloud disappeared. The cycle was repeated 3–4 times until reliable appearance and disappearance temperatures for the cloud were recorded.

Source and Purity of Materials:
(1) Source not specified; 99.8% by freezing point; main impurities are isomeric xylenes; used as received.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) *m*-Xylene; C_8H_{10} ; [108-38-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).

Variables:
Temperature: 15 °*C*–45 °C

Prepared By:
G. T. Hefter

Experimental Data

Solubility of *m*-xylene in water

t/°C	$10^5 \cdot x_1$ (compiler)[a]	*g*(1)/100 g sln (compiler)[a]	$10^3 \cdot$ mol(1)/L sln
15	2.68	0.0158	1.49 ± 0.04
25	2.75	0.0162	1.52 ± 0.06
35	2.85	0.0168	1.57 ± 0.10
45	3.15	0.0186	1.73 ± 0.08

[a]Assuming solution densities to be the same as those of pure water at the same temperature (Kell[1]).

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to an earlier design (Sanemasa *et al.*[2]) and is described in detail in the paper. 100–200 mL of (2) and 10–20 mL of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was established a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 mL aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.

Source and Purity of Materials:
(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 98.0%, used without further purification.
(2) Redistilled; no further details given.

Estimated Error:
Temperature: ±0.1 °C.
Solubility: see table, type of error not specified.

References:
[1]G. S. Kell, J. Chem. Eng. Data **20**, 97(1975).
[2]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Chem. Lett. 225 (1981).

Components:
(1) *m*-Xylene; C_8H_{10} ; [108-38-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. Sanemasa, Y. Miyazaki, S. Arakawa, M. Kumamaru, and T. Deguchi, Bull. Chem. Soc. Jpn. **60**, 517 (1987).

Variables:
One temperature: 25.0 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of *m*-xylene in water

t/°C	mol (1)/L sln	g(1)/100 g sln (compilers)	x_1 (compilers)
25.0	$1.33 \cdot 10^{-3}$	$1.41 \cdot 10^{-2}$	$2.40 \cdot 10^{-5}$

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. The apparatus used for preparing aqueous solutions saturated with hydrocarbon vapor was the same as that previously reported in Sanemasa *et al.*[1] The method was based on the introduction of phase (1) (by bubbling air through the mixture using circulating pump in a closed system) into 100 mL of water. After 10 min (at circulation rate of vapor of 1.5 L/min) equilibrium was attained, and a 30 mL portion of the saturated aqueous solution was transferred into three separatory funnels with 5 mL of toluene. Mixtures were analyzed by gas chromatography.

Source and Purity of Materials:
(1) Source not specified; analytical reagent grade; purity 98%; used as received.
(2) Deionized and redistilled.

Estimated Error:
Temperature: ±0.1 °C

References:
[1]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).

Components:
(1) *m*-Xylene; C_8H_{10} ; [108-38-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
S. Sawamura, K. Suzuki, and Y. Taniguchi, J. Solution Chem. **16**, 649 (1987).

Variables:
One temperature: 25.00 °C
Pressure: 0.1 MPa–385 MPa

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of *m*-xylene in water

t/°C	P/MPa	x_p/x_0	g(1)/100 g sln (compilers)	$10^5 \cdot x_1$ (compilers)
25.00	0.1	1	0.01591	2.70, Ref. 2
	50	1.073	0.01709	2.90
	100	1.105	0.01756	2.98
	150	1.104	0.01756	2.98
	200	1.081	0.01721	2.92
	250	1.058	0.01685	2.86
	300	1.024	0.01626	2.76
	350	0.981	0.01561	2.65
	385	0.946	0.01503	2.55

x_p/x_0=relation of solubilities at high and normal pressure.

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. Water (2) and a few drops of hydrocarbon (1) were placed in a high pressure optical cell with a Teflon ball for stirring. The sample was pressurized and shaken in a thermoregutated water bath for 5–20 h. Details of the apparatus, procedures, and purification were reported in Sawamura *et al.*[1] Solubilities were calculated by the compilers on the basis of absorbance measurements and recommended solubility value at 25 °C and 0.1 MPa reported in Shaw.[2]

Source and Purity of Materials:
(1) Nakarai Chem. (Japan); shaken successively with H_2SO_4, NaOH, H_2O, dried over $CaCl_2$, distilled.
(2) Deionized; distilled with a trace of $KMnO_4$.

Estimated Error:
Temperature: ±0.05 °C.

References:
[1]S. Sawamura, M. Tsuchiya, Y. Taniguchi, and K. Suzuki, Physica **139**, 732 (1986).
[2]D. G. Shaw, ed., *IUPAC Solubility Data Series*, Vol. 38 (Pergamon, New York, 1989).

Components:	Original Measurements:
(1) *m*-Xylene; C_8H_{10} ; [108-38-3] (2) Water; H_2O; [7732-18-5]	C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and Z. Maczynska

Experimental Data

The solubility of *m*-xylene in water at 25 °C was reported to be 146.0 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.01460 $g(1)$/100 g sln and $2.48 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:

The concentration of (1) in (2) was determined by gas chromatography

Source and Purity of Materials:

(1) Aldrich Chemical Co. or Matheson, Coleman, and Bell 99+%.
(2) Distilled.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: 1.6 mg (1)/kg (2) (standard deviation of the mean for six replicates).

Components:	Original Measurements:
(1) *m*-Xylene; C_8H_{10} ; [108-38-3] (2) Water; H_2O; [7732-18-5]	Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).
Variables:	**Prepared By:**
One temperature: 25.0 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of *m*-xylene in water

t/°C	mol (1)/L sln	$g(1)$/100 g sln (compilers)	x_1 (compilers)
25.0	$1.51 \cdot 10^{-3}$	$1.61 \cdot 10^{-2}$	$2.73 \cdot 10^{-5}$

Auxiliary Information

Method/Apparatus/Procedure:

A generator column method was used, as described in DeVoe *et al.*[1] and May *et al.*[2] A column was coated with (1) by pulling about 2 mL of liquid through the clean dry support (Chromosorb W-HP). A saturated solution was generated by pumping water into the inlet of the coated column and was then analyzed by hplc. The column was thermostatted by pumping water from a bath through a column jacket. An average of at least three measurements is reported.

Source and Purity of Materials:

(1) Source not specified; purity >99 mole % checked by high temperature glc.
(2) Source not specified.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: 1% (estimated by the authors).

References:

[1]H. De Voe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. (USA) **86**, 361 (1981).
[2]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).

Components:
(1) *m*-Xylene; C_8H_{10} ; [108-38-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. Vesala, Acta Chem. Scand., Ser. A **28**, 839 (1974).

Variables:
One temperature: 298.15 K

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of *m*-xylene in water

T/K	mol(1)/g(2)	$g(1)$/100 g sln (compilers)	x_1 (compilers)
298.15	$(1.94\pm0.01)\cdot10^{-6}$	$2.06\cdot10^{-4}$	$3.49\cdot10^{-5}$

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. The equilibration was carried out in a modified vessel (Franks *et al.*[1]), equipped with a magnetic stirrer. The temperature of the water bath was maintained within ±0.05 K. Equilibrium was obtained after 48 h and then samples were analyzed by spectrophotometry. At least 5 parallel determinations were performed.

Source and Purity of Materials:
(1) Commercial analytical grade reagent; purity 99% by glc; distilled through a column.
(2) Distilled water passed through an Amberlite CG 20+CG 400 ion-exchange column.

Estimated Error:
Temperature: ±0.05 K.
Solubility: as above.

References:
[1]F. Franks, M. Gent, and H. H. Johnson, J. Chem. Soc. 2716 (1963).

2.5. *p*-Xylene+Water

Components:
(1) *p*-Xylene (1,4-dimethylbenzene); C_8H_{10} ; [106-42-3]
(2) Water; H_2O; [7732-18-5]

Evaluators:
A. Maczynski, M. Goral, and B. Wisniewska-Goclowska, Thermodynamics Data Center, Warsaw, Poland, January, 2004.

Critical Evaluation of the Solubility of *p*-Xylene (1) in Water (2)

The experimental solubility data for (1) in (2) have been investigated by the authors listed below together with temperature range and pressure range, if reported:

Author (s)	T/K	Author (s)	T/K
Andrews and Keefer[1]	298	Price[12]	298
Ben-Naim and Wilf[2]	283–293	Pryor and Jentoft[13]	316–568
Bohon and Claussen[3]	298	Sanemasa *et al.*[14]	288–318
Chen and Wagner[4]	303–373 (136–204 kPa)	Sanemasa *et al.*[15]	298
Guseva and Parnov[5]	414–531	Sawamura *et al.*[16]	298
Keeley *et al.*[8]	298	Sutton and Calder[17]	298
Lo *et al.*[10]	298	Tewari *et al.*[18]	298
Polak and Lu[11]	273 and 298		

Reference solubility data for (1) in (2) were obtained by the Evaluators using the procedures described in the Preface to Part 2 and expressed by the equation:

$$\ln x_1 = \ln x_{\min,1} + D[(T_{\min}/T)\ln(T_{\min}/T) + 1 - (T_{\min}/T)], \quad (1)$$

where $\ln x_{\min,1} = -10.56$, $D = 41.7$, and $T_{\min} = 290$.

Equation (1) is based on all available solubility data of hydrocarbons in water and is used for calculations of the Reference data. Comparison between Reference and experimental data is one of the criteria used to assign data to the categories listed in Table 14.

TABLE 14. The data categories for solubility of *p*-xylene (1) in water (2)

T/K	Recommended [data in good agreement (±30%) with each other and with the reference data]	Tentative [data in good agreement (±30%) with the reference data]	Doubtful [data in poor agreement (>30%) with the reference data]
273.2		Polak and Lu[11]	
283.2		Ben-Naim and Wilf[2]	
288.2		Sanemasa *et al.*[14]	
293.2		Ben-Naim and Wilf[2]	
298.1		Sanemasa *et al.*[15]	
298.2	Keeley *et al.*[8] Price[12] Sanemasa *et al.*[14] Sutton and Calder[17]	Andrews and Keefer[1] Bohon and Claussen[3] Lo *et al.*[10] Price[12] Sawamura *et al.*[16]	Tewari *et al.*[18]
303.2		Chen and Wagner[4]	
308.2		Sanemasa *et al.*[14]	
313.2		Chen and Wagner[4]	
316.2			Pryor and Jentoft[13]
318.2		Sanemasa *et al.*[14]	
323.2		Chen and Wagner[4]	
329.6			Pryor and Jentoft[13]
333.2		Chen and Wagner[4]	
338.2			Pryor and Jentoft[13]
343.2		Chen and Wagner[4]	
348.5			Pryor and Jentoft[13]
353.2		Chen and Wagner[4]	
360.4		Pryor and Jentoft[13]	

363.2	Chen and Wagner[4]	
373.2	Chen and Wagner[4]	
414.2		Guseva and Parnov[5]
435.7	Pryor and Jentoft[13]	
442.2		Guseva and Parnov[5]
461.3	Pryor and Jentoft[13]	
467.2		Guseva and Parnov[5]
504.2		Guseva and Parnov[5]
516.4	Pryor and Jentoft[13]	
531.2		Guseva and Parnov[5]
555.7	Pryor and Jentoft[13]	
567.7		Pryor and Jentoft[13]

All the experimental and reference data are listed in Table 15 and shown in Fig. 12. The Recommended and Tentative data are shown in Fig. 13.

TABLE 15. Experimental values for solubility of *p*-xylene (1) in water (2)

T/K	*P*/kPa	Experimental values x_1 (R=recommended, T=tentative, D=doubtful)	Reference values $x_1 \pm 30\%$
273.2		$2.78 \cdot 10^{-5}$ (T; Ref. 11)	$2.8 \cdot 10^{-5}$
283.2		$3.21 \cdot 10^{-5}$ (T; Ref. 2)	$2.6 \cdot 10^{-5}$
288.2		$2.67 \cdot 10^{-5}$ (T; Ref. 14)	$2.6 \cdot 10^{-5}$
293.2		$3.25 \cdot 10^{-5}$ (T; Ref. 2)	$2.6 \cdot 10^{-5}$
298.1		$2.73 \cdot 10^{-5}$ (T; Ref. 15)	$2.6 \cdot 10^{-5}$
298.2		$3.39 \cdot 10^{-5}$ (T; Ref. 1), $3.36 \cdot 10^{-5}$ (T; Ref. 3), $2.95 \cdot 10^{-5}$ (R; Ref. 8), $3.20 \cdot 10^{-5}$ (T; Ref. 10), $3.14 \cdot 10^{-5}$ (T; Ref. 11), $2.66 \cdot 10^{-5}$ (R; Ref. 12), $2.76 \cdot 10^{-5}$ (R; Ref. 14), $2.65 \cdot 10^{-5}$ (R; Ref. 17), $2.07 \cdot 10^{-5}$ (T; Ref. 16), $3.65 \cdot 10^{-5}$ (D; Ref. 18)	$2.6 \cdot 10^{-5}$
303.2	136 (Ref. 4)	$2.86 \cdot 10^{-5}$ (T; Ref. 4)	$2.7 \cdot 10^{-5}$
308.2		$2.92 \cdot 10^{-5}$ (T; Ref. 14)	$2.8 \cdot 10^{-5}$
313.2	136 (Ref. 4)	$3.18 \cdot 10^{-5}$ (T; Ref. 4)	$2.9 \cdot 10^{-5}$
316.2		$4.34 \cdot 10^{-5}$ (D; Ref. 13)	$3.0 \cdot 10^{-5}$
318.2		$3.02 \cdot 10^{-5}$ (T; Ref. 14)	$3.1 \cdot 10^{-5}$
323.2	136 (Ref. 4)	$3.44 \cdot 10^{-5}$ (T; Ref. 4)	$3.3 \cdot 10^{-5}$
329.6		$5.10 \cdot 10^{-5}$ (D; Ref. 13)	$3.5 \cdot 10^{-5}$
333.2	136 (Ref. 4)	$4.04 \cdot 10^{-5}$ (T; Ref. 4)	$3.7 \cdot 10^{-5}$
338.2		$5.76 \cdot 10^{-5}$ (D; Ref. 13)	$4.0 \cdot 10^{-5}$
343.2	136 (Ref. 4)	$4.83 \cdot 10^{-5}$ (T; Ref. 4)	$4.4 \cdot 10^{-5}$
348.5		$6.56 \cdot 10^{-5}$ (D; Ref. 13)	$4.8 \cdot 10^{-5}$
353.2	136 (Ref. 4)	$5.71 \cdot 10^{-5}$ (T; Ref. 4)	$5.3 \cdot 10^{-5}$
360.4		$7.79 \cdot 10^{-5}$ (T; Ref. 13)	$6.1 \cdot 10^{-5}$
363.2	170 (Ref. 4)	$6.70 \cdot 10^{-5}$ (T; Ref. 4)	$6.4 \cdot 10^{-5}$
373.2	204 (Ref. 4)	$8.74 \cdot 10^{-5}$ (T; Ref. 4)	$7.9 \cdot 10^{-5}$
414.2		$8.30 \cdot 10^{-5}$ (D; Ref. 5)	$2.1 \cdot 10^{-4}$
435.7		$4.264 \cdot 10^{-4}$ (T; Ref. 13)	$3.6 \cdot 10^{-4}$
442.2		$1.63 \cdot 10^{-4}$ (D; Ref. 5)	$4.3 \cdot 10^{-4}$
461.3		$7.686 \cdot 10^{-4}$ (T; Ref. 13)	$7.1 \cdot 10^{-4}$
467.2		$3.93 \cdot 10^{-4}$ (D; Ref. 5)	$8.3 \cdot 10^{-4}$
504.2		$1.034 \cdot 10^{-3}$ (D; Ref. 5)	$2.2 \cdot 10^{-3}$
516.4		$2.956 \cdot 10^{-3}$ (T; Ref. 13)	$3.1 \cdot 10^{-3}$
531.2		$2.20 \cdot 10^{-3}$ (D; Ref. 5)	$4.5 \cdot 10^{-3}$
555.7		$7.624 \cdot 10^{-3}$ (T; Ref. 13)	$8.4 \cdot 10^{-3}$
567.7		$7.541 \cdot 10^{-3}$ (D; Ref. 13)	$1.1 \cdot 10^{-2}$

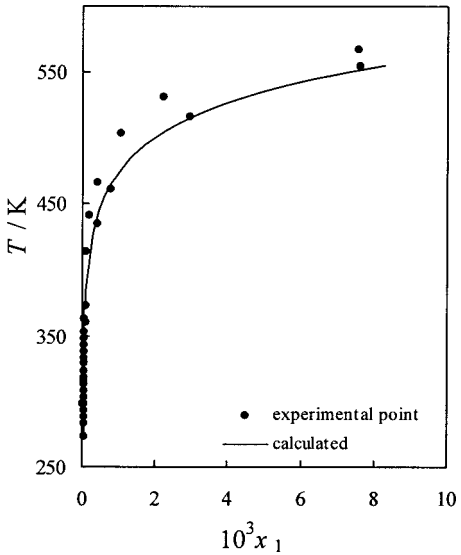

FIG. 12. All the solubility data for *p*-xylene (1) in water (2).

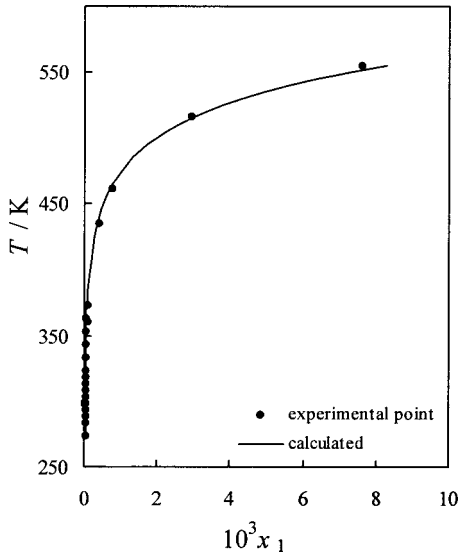

FIG. 13. Recommended and tentative solubility data for *p*-xylene (1) in water (2).

Critical Evaluation of the Solubility of Water (2) in *p*-Xylene (1)

The experimental solubility data for (2) in (1) have been investigated by the authors listed below together with temperature range and pressure range, if reported:

Author (s)	*T*/K	Author (s)	*T*/K
Chen and Wagner[4]	303–373 (136–204 kPa)	Kirchnerova and Cave[9]	298
Högfeldt and Bolander[7]	298	Polak and Lu[11]	298

Reference solubility data for (2) in (1) were obtained by the Evaluators using the method described in the Preface to Part 2 and expressed by the equation:

$$\ln x_2 = d_1 + d_2(1/T_r - 1) + d_3(1 - T_r)^{1/3} + d_4(1 - T_r), \quad (2)$$

where $d_1 = -0.386$, $d_2 = -3.206$, $d_3 = -0.003$, $d_4 = -5.597$, and $T_r = T/566.4$.

Equation (2) was used for obtaining the Reference data by regression of the data obtained from those calculated from Reference data of solubility of *p*-xylene in water by the Equation of State with an association term. Comparison between Reference and experimental data is one of the criteria used to assign data to categories.

All the experimental and reference solubility data for (2) in (1) are listed in Table 16 and shown in Fig. 14. The data of Högfeldt and Bolander,[7] Kirchnerova and Cave,[9] and Polak and Lu[11] at 298 K are in good agreement (within 30% relative standard deviation) with each other and with the reference data and are Recommended. The data of Chen and Wagner[4] are in good agreement (within 30% relative standard deviation) with the reference data and are Tentative. The Recommended and Tentative data are shown in Fig. 4.

TABLE 16. Experimental values for solubility of water (2) in *p*-xylene (1)

T/K	*P*/kPa	Experimental values x_2 (R=recommended, T=tentative, D=doubtful)	Reference values $x_2 \pm 30\%$
298.2		$2.70 \cdot 10^{-3}$ (R; Ref. 7), $2.69 \cdot 10^{-3}$ (R; Ref. 9), $2.59 \cdot 10^{-3}$ (R; Ref. 11)	$2.7 \cdot 10^{-3}$
303.2	136 (Ref. 4)	$2.71 \cdot 10^{-3}$ (T; Ref. 4)	$3.1 \cdot 10^{-3}$
313.2	136 (Ref. 4)	$3.48 \cdot 10^{-3}$ (T; Ref. 4)	$4.2 \cdot 10^{-3}$
323.2	136 (Ref. 4)	$4.75 \cdot 10^{-3}$ (T; Ref. 4)	$5.5 \cdot 10^{-3}$
333.2	136 (Ref. 4)	$6.51 \cdot 10^{-3}$ (T; Ref. 4)	$7.2 \cdot 10^{-3}$
343.2	136 (Ref. 4)	$8.70 \cdot 10^{-3}$ (T; Ref. 4)	$9.3 \cdot 10^{-3}$
353.2	136 (Ref. 4)	$1.15 \cdot 10^{-2}$ (T; Ref. 4)	$1.2 \cdot 10^{-2}$
363.2	170 (Ref. 4)	$1.57 \cdot 10^{-2}$ (T; Ref. 4)	$1.5 \cdot 10^{-2}$
373.2	204 (Ref. 4)	$2.02 \cdot 10^{-2}$ (T; Ref. 4)	$1.9 \cdot 10^{-2}$

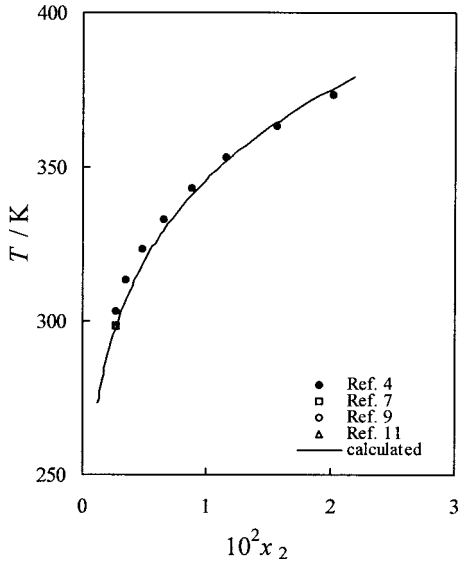

FIG. 14. All the solubility data for water (2) in *p*-xylene (1).

High Pressure Solubility of *p*-Xylene (1) in Water (2)

The experimental high pressure solubility for (1) in (2) investigated by the Haruki *et al.*[6] at 553 and 583 K and 10 200–26 500 kPa, and Sawamura *et al.*[16] at 298 K and 50 000 kPa has not been critically evaluated because the developed method is not applied for such data.

An evaluation of these data was presented by Hefter and Young.[71]

Rejected and Inaccessible Data

In the opinion of the evaluators uncertainty exists as to whether the solubility measurements reported by Krzyzanowska and Szeliga[19] are independent data. Therefore these data are Rejected.

Refereces:

[1]L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **71**, 3644 (1949).
[2]A. Ben-Naim and J. Wilf, J. Chem. Phys. **70**, 771 (1979).
[3]R. L. Bohon and W. F. Claussen, J. Am. Chem. Soc. **73**, 1571 (1951).
[4]H. Chen and J. Wagner, J. Chem. Eng. Data **39**, 679 (1994).
[5]A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **18**, 76 (1963).
[6]M. Haruki, Y. Iwai, S. Nagao, and Y. Arai, J. Chem. Eng. Data **46**, 950 (2001).
[7]E. Högfeldt and B. Bolander, Ark. Kemi **21**, 161 (1964).
[8]D. F. Keeley, M. A. Hoffpauir, and J. R. Meriwether, J. Chem. Eng. Data **36**, 456 (1991).
[9]J. Kirchnerova and G. C. B. Cave, Can. J. Chem. **54**, 3909 (1976).
[10]J. M. Lo, C. L. Tseng, and J. Y. Yang, Anal. Chem. **58**, 1596 (1986).
[11]J. Polak and B. C. Y. Lu, Can. J. Chem. **51**, 4018 (1973).
[12]L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).
[13]W. A. Pryor and R. E. Jentoft, J. Chem. Eng. Data **6**, 36 (1961).
[14]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).
[15]I. Sanemasa, Y. Miyazaki, S. Arakawa, M. Kumamaru, and T. Deguchi, Bull. Chem. Soc. Jpn. **60**, 517 (1987).
[16]S. Sawamura, K. Suzuki, and Y. J. Taniguchi, J. Solution Chem. **16**, 649 (1987).
[17]C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).
[18]Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).
[19]T. Krzyzanowska and J. Szeliga, Nafta (Katowice) **12**, 413 (1978).

Components:
(1) *p*-Xylene; C_8H_{10} ; [106-42-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **71**, 3644 (1949).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

The solubility of *p*-xylene in water at 25 °C was reported to be 0.0200 g (1)/100 g sln.

The corresponding mole fraction, x_1 , calculated by the compilers is $3.39 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:
A mixture of (1) and (2) was rotated for 20 h in a constant temperature bath at 25 °C. A sample (5–20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10–50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

Source and Purity of Materials:
(1) Eastman Kodak Co. best grade; fractionally distilled; b.p. 138.5 °C.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) *p*-Xylene; C_8H_{10} ; [106-42-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. Ben-Naim and J. Wilf, J. Phys. Chem. **70**, 771 (1979).

Variables:
Temperature: 10.0 °C and 20.0 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of *p*-xylene in water

t/°C	$10^3 \cdot$ mol(1)/L sln	$10^2 \cdot g(1)$/100 g sln (compilers)	$10^5 \cdot x_1$ (compilers)
10.0	1.78	1.89	3.21
20.0	1.80	1.91	3.25

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. A saturated solution was diluted several times and the optical density was measured by a Perkin-Elmer Model 450 spectrophotometer in the UV region of 200–400 nm.

Source and Purity of Materials:
(1) Fluka, puriss grade, purity ⩾99.5%; used as received.
(2) Triply distilled.

Estimated Error:
Temperature: ±0.2 °C.
Solubility: 1% (reproducibility of measurements).

Components:
(1) *p*-Xylene; C_8H_{10} ; [106-42-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. L. Bohon and W. F. Claussen, J. Am. Chem. Soc. **73**, 1571 (1951).

Variables:
Temperature: 0.4 °C–42.8 °C

Prepared By:
G. T. Hefter

Experimental Data

Solubility of *p*-xylene in water

t/°C	$10^5 \cdot x_1$ (compiler)	$g(1)$/100 g sln[a] (compiler)
0.4	2.64[b]	0.0150[b]
10.0	3.19[b]	0.0188[b]
10.0	3.34	0.0197
14.9	3.31	0.0195
21.0	3.34	0.0197
25.0	3.36[c]	0.0198[c]
25.6	3.37	0.0199
30.2	3.41	0.0201
30.3	3.46	0.0204
34.9	3.51	0.0207
35.2	3.51	0.0207
42.8	3.76	0.0222

[a]Solubilities of (1) in (2) were reported as ''optical density'' (absorbance) measurements. Solubilities were calculated by the compiler using the Beer-Lambert law, the stated cell path length (1 cm) and the authors' ''extinction coefficients'' (absorptivities) and corrected optical densities. This gave a solubility of $g(1)$/L sln which was then converted to $g(1)$/100 g sln by assuming a solution density of 1.00 kg/L.

[b]Data refer to solubility solid (1) in (2).

[c]Given in the original paper as 0.198 $g(1)$/L sln.

Auxiliary Information

Method/Apparatus/Procedure:
A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24 h and then allowed to settle for at least another 24 h. Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been tarred, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of the samples were inserted into a quartz cuvette and measured in a Beckman DU spectrophotometer. Absorbances were corrected for adsorption of (1) onto the walls of the cuvette.

Source and Purity of Materials:
(1) Eastman Kodak Co., purified by recrystallization from ethanol, washing, filtering through silica gel then distilling. Purity was determined by refractometry (no details given).
(2) Air-free conductivity water (no details given).

Estimated Error:
Temperature: ±0.02 °C.
Solubility: ±0.5% relative.

Components:
(1) *p*-Xylene; C_8H_{10} ; [106-42-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. Chen and J. Wagner, J. Chem. Eng. Data **39**, 679 (1994).

Variables:
Temperature: 303.15 K–373.15 K
Pressure: 1.36 bar and 2.04 bar

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of *p*-xylene in water

T/K	P/bar	$g(1)$/100 g sln (compilers)	$10^5 \cdot x_1$
303.15	1.36	0.0168	2.86±0.06
313.15	1.36	0.0187	3.18±0.15
323.15	1.36	0.0202	3.44±0.07
333.15	1.36	0.0238	4.04±0.05
343.15	1.36	0.0284	4.83±0.06
353.15	1.36	0.0336	5.71±0.07
363.15	1.70	0.0394	6.70±0.10
373.15	2.04	0.0514	8.74±0.22

Solubility of water in *p*-xylene

T/K	P/bar	$g(2)$/100 g sln (compilers)	$10^2 \cdot x_2$
303.15	1.36	0.0461	0.271±0.009
313.15	1.36	0.0592	0.348±0.020
323.15	1.36	0.0809	0.475±0.016
333.15	1.36	0.1111	0.651±0.047
343.15	1.36	0.1487	0.870±0.075
353.15	1.36	0.1970	1.15±0.073
363.15	1.70	0.2699	1.57±0.063
373.15	2.04	0.3486	2.02±0.107

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. The continuous flow equilibrium apparatus for mutual solubility measurements, Chen and Wagner,[1] was used. Samples were collected in 25 mL vials and 60 and 120 mL bottles containing anhydrous ethanol or dichloromethane as a solvent. Details of the standard preparation, calibration, and sampling procedures were described in Chen and Wagner.[2] A Hewlett-Packard 5880A gas chromatograph equipped with Porapac Q or GlasChrom 254 columns and a thermal conductivity detector was used for analysis. Reported solubilities are the average of 4–6 replicate determinations.

Source and Purity of Materials:
(1) Aldrich Chemical Co.; HPLC grade, purity 99.5 mole %, used as received.
(2) Distilled and deionized water.

Estimated Error:
Temperature: ±0.2 K.
Solubility: standard deviation as above.

References:
[1]H. Chen and J. Wagner, J. Chem. Eng. Data **39**, 470 (1994)
[2]H. Chen and J. Wagner, J. Chem. Eng. Data **39**, 475 (1994).

Components:
(1) *p*-Xylene; C_8H_{10} ; [106-42-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
M. Haruki, Y. Iwai, S. Nagao, and Y. Arai, J. Chem. Eng. Data **46**, 950 (2001).

Variables:
Temperature: 553.2 K and 583.2 K
Pressure: 10.2 MPa–26.5 MPa

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Mutual solubility of *p*-xylene in water

T/K	*P*/MPa	*g*(1)/100 g sln (compilers)	x_1
553.2	10.2	0.029	0.005±0.0009
	14.3	0.040	0.007±0.0005
	17.4	0.040	0.007±0.0006
	20.4	0.034	0.006±0.0007
	23.5	0.034	0.006±0.0005
	26.5	0.040	0.007±0.0004
583.2	17.3	0.097	0.018±0.0010
	20.4	0.087	0.016±0.0013
	23.2	0.092	0.017±0.0013
	26.2	0.092	0.017±0.0009

Mutual solubility of water in *p*-xylene

T/K	*P*/MPa	*g*(2)/100 g sln (compilers)	x_2
553.2	10.2	15.6	0.522±0.0124
	14.3	14.4	0.497±0.0064
	17.4	13.5	0.480±0.0066
	20.4	12.4	0.456±0.0045
	23.5	12.4	0.456±0.0104
	26.5	10.7	0.415±0.0122
583.2	12.9	39.0	0.790±0.0058
	14.7	33.3	0.746±0.0074
	17.3	30.7	0.723±0.0052
	20.4	28.2	0.698±0.0037
	23.2	26.9	0.684±0.0085
	26.2	23.8	0.648±0.0071

Auxiliary Information

Method/Apparatus/Procedure:
A flow-type apparatus to measure the phase equilibria at high temperatures and pressures was used, details were described in Haruki *et al.*[1] Pressure was controlled by back-pressure regulators. The phase behavior was observed with a video camera attached to a telescope. Samples of each phase were collected in bottles containing ethanol to obtain homogenous solutions. The compositions of samples were analyzed by a gas chromatograph with a thermal conductivity detector. Solubilities reported above are the arithmetic average of 8–16 experimental points.

Source and Purity of Materials:
(1) Wako Pure Chem. Ind.; purity >98 mole % by glc; used as received.
(2) Distilled water was purified by Milliq-Labo (Millipore Co,) equipment.

Estimated Error:
Temperature: ±1 K.
Pressure: ±0.1 MPa.

References:
[1]M. Haruki, Y. Iwai, S. Nagao, Y. Yahiro, and Y. Arai, J. Chem. Eng. Res. **39**, 4516 (2000).

Components:
(1) *p*-Xylene; C_8H_{10} ; [106-42-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. N. Guseva and E. I. Parnov, Vestn. Mosk. Univ., Ser. 2: Khim. **18**, 76 (1963).

Variables:
Temperature: 141 °C–258 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

Solubility of *p*-xylene in water

t/°C	$10^4 \cdot x_1$ (compiler)	*g*(1)/100 g sln
141	0.83	0.049
169	1.63	0.096
194	3.93	0.231
231	10.34	0.607
258	22.00	1.283

Auxiliary Information

Method/Apparatus/Procedure:
The measurements were made in sealed glass tubes. No details were reported in the paper.

Source and Purity of Materials:
(1) Source not specified; $n_D^{20}=1.4958$
(2) Doubly distilled.

Estimated Error:
Not specified.

Components:
(1) *p*-Xylene; C_8H_{10} ; [106-42-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
E. Högfeldt and B. Bolander, Ark. Kemi **21**, 161 (1964).

Variables:
One temperature: 25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

The solubility of water in *p*-xylene was reported to be 0.022 mol (2)/L sln.

The corresponding mass percent and mol fraction, x_2 , calculated by the compilers are $0.045g(2)$/100 g sln and 0.0027. The assumption that 1.00 L sln=857 g sln was used in the calculation.

Auxiliary Information

Method/Apparatus/Procedure:
The water determination was carried out according to Johansson's modification of the Karl Fischer titration described in Hardy *et al.*[1] and Johansson.[2]

Source and Purity of Materials:
(1) Fluka; 0.04% of ethylbenzene; purity 99.8%; used as received.
(2) Not specified

Estimated Error:
Temperature: ±0.3 °C.
Solubility: ±0.002 mol(2)/L sln (type of error not specified).

References:
[1]C. J. Hardy, B. F. Greenfield, and D. Scargill, J. Chem Soc. 90 (1961).
[2]A. Johansson, Sv. Papperstidn. **11B**, 124 (1947).

Components:
(1) *p*-Xylene; C_8H_{10} ; [106-42-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
D. F. Keeley, M. A. Hoffpauir, and J. R. Meriwether, J. Chem. Eng. Data **36**, 456 (1991).

Variables:
One temperature: 298.15 K

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of *p*-xylene in water

T/K	mol(1)/L sln	$g(1)$/100 g sln (compilers)	x_1 (compilers)
298.15	$(1.63\pm0.02)\cdot10^{-3}$	$1.74\cdot10^{-2}$	$2.95\cdot10^{-5}$

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was determined by a headspace chromatographic analysis, Keeley and Meriwether,[1] using a multiple injection interrupted flow technique. Samples were prepared in septum bottles of 160 mL volume which were thermostatted and shaken for 72 h prior to analysis. For analysis each bottle was transferred to a tempering beaker and pressurized to 15.00 psig with chromatographic grade nitrogen. Bottles were attached to the headspace sampling port of a chromatograph with 1 m by 3.2 mm stainless steel column (5% SP-1200, 1.75% Bentone-34) on 100/1200 mesh Supelcoport (Supelco Inc.) and FID detector. Solubility was calculated on the basis of Henry's law.

Source and Purity of Materials:
(1) Two samples were used: Baker, purity 99.78% checked by glc, used as received, and Aldrich Gold Label; purity 99.83% checked by glc, used as received.
(2) Deionized water.

Estimated Error:
Temperature: ±0.05 K.

References:
[1]D. F. Keeley and J. R. Meriwether, Rev. Sci. Instrum. **57**, 1434 (1986).

Components:	**Original Measurements:**
(1) *p*-Xylene; C_8H_{10} ; [106-42-3] (2) Water; H_2O; [7732-18-5]	J. Kirchnerova and G. C. B. Cave, Can. J. Chem. **54**, 3909 (1976).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and Z. Maczynska

Experimental Data

The solubility of water in *p*-xylene at 25 °C was reported to be 0.0217 mol (2)/L and $x_2 = 0.00269$.

The corresponding mass percent calculated by the compilers is 0.0457 $g(2)$/100 g sln.

Auxiliary Information

Method/Apparatus/Procedure:

Approximately 50 mL of (1) was placed in the equilibration vessel. A test tube containing 6 mL of (2) was then placed in the vessel so that the rim of the test tube rested against the upper inside wall of the vessel. The vessel was then stoppered, placed inside a plastic bag, and the jacketed vessel was immersed up to its neck in a water thermostat. Trials had shown that the stoichiometric concentration of (1) in (2) became constant within 2 days.

The stoichiometric concentration of water was determined by a conventional Karl Fischer dead-stop back-titration.

Source and Purity of Materials:

(1) Fisher 277; purified by double crystallization.
(2) Not specified.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: 0.0002 mol (2)/L sln (standard deviation from 5 determinations).

Components:	**Original Measurements:**
(1) *p*-Xylene; C_8H_{10} ; [106-42-3] (2) Water; H_2O; [7732-18-5]	J. M. Lo, C. L. Tseng, and J. Y. Yang, Anal. Chem. **58**, 1596 (1986).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of *p*-xylene in water

t/°C	$g(1)$/100 g sln	x_1 (compilers)
25	0.019±0.001	$3.2 \cdot 10^{-5}$

Auxiliary Information

Method/Apparatus/Procedure:

The radiometric method was used. The radioagent, 1-pyrrolidinecarbodithioic acid cobalt salt labeled ^{60}Co, was first dissolved in component (1) before pure water was added. Both of the liquids were placed in a 1000 mL separation funnel. The mixture was shaken for 5 min and allowed to separate for next 30 min. Concentration was calculated from activity measurements by a NaI(Tl) scintillation detector.

Source and Purity of Materials:

(1) E. Merck; purity not specified.
(2) Demineralized and degassed.

Estimated Error:

Solubility: as above (standard deviation of mean).

Components:
(1) *p*-Xylene; C_8H_{10} ; [106-42-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. Polak and B. C.-Y. Lu, Can. J. Chem. **51**, 4018 (1973).

Variables:
Temperature: 0 °C–25 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

Solubility of *p*-xylene in water

t/°C	$10^5 \cdot x_1$ (compiler)	*g*(1)/100 g sln (compiler)	mg (1)/kg (2)
0[†a]	2.78	0.0164	164[c]
25[b]	3.14	0.0185	185[c]

Solubility of water in *p*-xylene

t/°C	$10^3 \cdot x_2$ (compiler)	*g*(2)/100 g sln (compiler)	mg (1)/kg (2)
25[b]	2.59	0.0440	440[c]

[a–c]See Estimated Error.

[†]*p*-xylene was at supercooled liquid phase.

Auxiliary Information

Method/Apparatus/Procedure:
Approximately 50 mL of (1) together with (2) were placed in a 125 mL Hypo-vial that was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 h and left in the bath for 3 days or was kept in the bath without stirring for 7 days, before samples were taken for analysis.
The solubility of water in the organic layer was determined by the Karl Fischer titration and the solubility of hydrocarbon in the water layer was determined by gas chromatography.

Source and Purity of Materials:
(1) Eastman Organics, pure grade reagent; shaken three times with distilled water.
(2) Distilled.

Estimated Error:
Temperature: (a) ±0.02 °C, (b) ±0.01 °C.
Solubility: (c) ±1.7% (from two or three determinations).

Components:
(1) *p*-Xylene; C_8H_{10} ; [106-42-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
L. C. Price, Am. Assoc. Pet. Geol. Bull. **60**, 213 (1976).

Variables:
One temperature: 25 °C

Prepared By:
M. C. Haulait-Pirson

Experimental Data

The solubility of *p*-xylene in water at 25°C and at system pressure was reported to be 157.0 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 0.0157 *g*(1)/100 g sln and $2.66 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and ensured saturation of the (2) phase in 2–4 days. Analyses were carried out by glc using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

Source and Purity of Materials:
Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.
(2) Distilled.

Estimated Error:
Temperature: ±1 °C.
Solubility: ±1.0 mg(1)/kg(2).

Components:
(1) *p*-Xylene; C_8H_{10} ; [106-42-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. A. Pryor and R. E. Jentoft, J. Chem. Eng. Data **6**, 36 (1961).

Variables:
Temperature: 43.0 °C–294.5 °C

Prepared By:
A. Maczynski and Z. Maczynska

Experimental Data

Solubility of *p*-xylene in water

t/°C	$10^3 \cdot x_1$	g(1)/100 g sln (compiler)
43.0	0.0434	0.0256
56.4	0.0510	0.0301
65.0	0.0576	0.0340
75.3	0.0656	0.0387
87.2	0.0779	0.0459
162.5	0.4264	0.2508
188.1	0.7686	0.4514
243.2	2.9555	1.7174
282.5	7.6238	4.3326
294.5	7.5407	4.2871

Auxiliary Information

Method/Apparatus/Procedure:
Mixtures of (1) and (2) were carefully weighed into glass ampoules. The ampoules were sealed allowing just enough space for thermal expansion. The ampoule, observed through a telescope from behind a safety barrier, was suspended in a 4 L stirred silicone oil bath, and the bath was heated until the (1) dissolved. On cooling, a cloud of fine (1) droplets appeared, making the suspension opaque. The temperature was raised until the cloud disappeared. The cycle was repeated 3–4 times until reliable appearance and disappearance temperatures for the cloud were recorded.

Source and Purity of Materials:
(1) Source not specified; 99.1% by freezing point; main impurities are isomeric xylenes; used as received.
(2) Not specified.

Estimated Error:
Not specified.

Components:
(1) *p*-Xylene; C_8H_{10} ; [106-42-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).

Variables:
Temperature: 15 °C–45 °C

Prepared By:
G. T. Hefter

Experimental Data

Solubility of *p*-xylene in water

t/°C	$10^5 \cdot x_1$ (compiler)[a]	g(1)/100 g sln (compiler)[a]	$10^3 \cdot$ mol(1)/L sln
15	2.67	0.0157	1.48[b]
25	2.76	0.0163	1.53 ± 0.07
35	2.92	0.0172	1.61 ± 0.08
45	3.02	0.0178	1.66 ± 0.05

[a]Assuming solution densities to be the same as those of pure water at the same temperature (Kell[1]).
[b]No error given.

Auxiliary Information

Method/Apparatus/Procedure:
The apparatus is similar to an earlier design (Sanemasa *et al.*[2]) and is described in detail in the paper. 100–200 mL of (2) and 10–20 mL of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was established a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 mL aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.

Source and Purity of Materials:
(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 98.0%, used without further purification.
(2) Redistilled; no further details given

Estimated Error:
Temperature: ± 0.1 °C.
Solubility: see table, type of error not specified.

References:
[1]G. S. Kell, J. Chem. Eng. Data **20**, 97 (1975).
[2]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Chem. Lett. 225 (1981).

Components:
(1) *p*-Xylene; C_8H_{10} ; [106-42-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
I. Sanemasa, Y. Miyazaki, S. Arakawa, M. Kumamaru, and T. Deguchi, Bull. Chem. Soc. Jpn. **60**, 517 (1987).

Variables:
One temperature: 25.0 °C

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of *p*-xylene in water

t/°C	mol (1)/L sln	g(1)/100 g sln (compilers)	x_1 (compilers)
25.0	$1.51 \cdot 10^{-3}$	$1.61 \cdot 10^{-2}$	$2.73 \cdot 10^{-5}$

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. The apparatus used for preparing aqueous solutions saturated with hydrocarbon vapor was the same as that previously reported in Sanemasa *et al.*[1] The method was based on the introduction of phase (1) (by bubbling air through the mixture using circulating pump in a closed system) into 100 mL of water. After 10 min (at circulation rate of vapor of 1.5 L/min) equilibrium was attained, and a 30 mL portion of the saturated aqueous solution was transferred into three separatory funnels with 5 mL of toluene. Mixtures were analyzed by gas chromatography.

Source and Purity of Materials:
(1) Source not specified; analytical reagent grade; purity 98%; used as received.
(2) Deionized and redistilled.

Estimated Error:
Temperature: ±0.1 °C.

References:
[1]I. Sanemasa, M. Araki, T. Deguchi, and H. Nagai, Bull. Chem. Soc. Jpn. **55**, 1054 (1982).

Components:
(1) *p*-Xylene; C_8H_{10} ; [106-42-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
S. Sawamura, K. Suzuki, and Y. Taniguchi, J. Solution Chem. **16**, 649 (1987).

Variables:
One temperature: 25.00 °C
Pressure: 0.1–50 MPa

Prepared By:
A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of *p*-xylene in water

t/°C	P/MPa	x_p/x_0	g(1)/100 g sln (compilers)	$10^5 \cdot x_1$ (compilers)
25.00	0.1	1	0.0220	3.74
	50	1.086	0.0239	4.06

x_p/x_0=relation of solubilities at high and normal pressure.

Auxiliary Information

Method/Apparatus/Procedure:
The analytical method was used. Water (2) and a few drops of hydrocarbon (1) were placed in a high pressure optical cell with a Teflon ball for stirring. The sample was pressurized and shaken in a thermoregutated water bath for 5–20 h. Details of the apparatus, procedures, and purification were reported in Sawamura *et al.*[1] Solubilities were calculated by the compilers on the basis of absorbance measurements and the solubility value at 25 °C and 0.1 MPa.

Source and Purity of Materials:
(1) Nakarai Chem. (Japan); shaken successively with H_2SO_4, NaOH, H_2O, dried over $CaCl_2$, distilled.
(2) Deionized; distilled with a trace of $KMnO_4$.

Estimated Error:
Temperature: ±0.05 °C.

References:
[1]S. Sawamura, M. Tsuchiya, Y. Taniguchi, and K. Suzuki, Physica **139**, 732 (1986).

Components:	Original Measurements:
(1) *p*-Xylene; C_8H_{10} ; [106-42-3] (2) Water; H_2O; [7732-18-5]	C. Sutton and J. A. Calder, J. Chem. Eng. Data **20**, 320 (1975).
Variables:	**Prepared By:**
One temperature: 25 °C	A. Maczynski and Z. Maczynska

Experimental Data

The solubility of *p*-xylene in water at 25 °C was reported to be 156.0 mg (1)/kg (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.01560 $g(1)$/100 g sln and $2.65 \cdot 10^{-5}$.

Auxiliary Information

Method/Apparatus/Procedure:

The concentration of (1) in (2) was determined by gas chromatography.

Source and Purity of Materials:

(1) Aldrich Chemical Co. or Matheson, Coleman, and Bell 99+%
(2) Distilled.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: 1.6 mg (1)/kg (2) (standard deviation of the mean for six replicates).

Components:	Original Measurements:
(1) *p*-Xylene; C_8H_{10} ; [106-42-3] (2) Water; H_2O; [7732-18-5]	Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).
Variables:	**Prepared By:**
One temperature: 25.0 °C	A. Skrzecz, I. Owczarek, and K. Blazej

Experimental Data

Solubility of *p*-xylene in water

t/°C	mol (1)/L sln	$g(1)$/100 g sln (compilers)	x_1 (compilers)
25.0	$2.02 \cdot 10^{-3}$	$2.15 \cdot 10^{-2}$	$3.65 \cdot 10^{-5}$

Auxiliary Information

Method/Apparatus/Procedure:

A generator column method was used, as described in DeVoe *et al.*[1] and May *et al.*[2] A column was coated with (1) by pulling about 2 mL of liquid through the clean dry support (Chromosorb W-HP). A saturated solution was generated by pumping water into the inlet of the coated column and was then analyzed by hplc and glc. The column was thermostatted by pumping water from a bath through a column jacket. An average of at least three measurements is reported.

Source and Purity of Materials:

(1) Source not specified; purity >99 mole % checked by high temperature glc.
(2) Source not specified.

Estimated Error:

Temperature: ±0.1 °C.
Solubility: 1% (estimated by the authors).

References:

[1]H. De Voe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. (USA) **86**, 361 (1981).
[2]W. E. May, S. P. Wasik, and D. H. Freeman, Anal. Chem. **50**, 175 (1978).

3. System Index

Page numbers preceded by E refer to evaluation text whereas those not preceded by E refer to compiled tables.

4. Registry Number Index

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5. Author Index

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